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GC/MS (Gas Chromatography-Mass Spectrometry) Analysis of Organics in Drinking Water Concentrates and Advanced Waste Treatment Concentrates. Volume 3

Battelle Columbus Labs., OH

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GC/MS ANALYSIS OF ORGANICS IN DRINKING WATER CONCENTRATES AND ADVANCED WASTE TREATMENT CONCENTRATES

Volume 3

Batch Liquid-Liquid Extraction and Analysis of 10-Liter Sample and Analysis of Concentrates from Small Volumes (10 to 50 Liters) of Drinking Water

by

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Contract No. 68-03-2548

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FOREWORD

The many benefits of our modern, developing, industrial society are accompanied by certain hazards. Careful assessment of the relative risk of existing and new man-made environmental hazards is necessary for the establishment of sound regulatory policy. These regulations serve to enhance the quality of our environment in order to promote the public health and welfare and the productive capacity of our Nation's population.

The complexities of environmental problems originate in the deep interdependent relationships between the various physical and biological segments of man's natural and social world. Solutions to these environmental problems require an integrated program of research and development using input from a number of disciplines. The Health Effects Research Laboratory, Research Triangle Park, NC and Cincinnati, OH conducts a coordinated environmental health research program in toxicology, epidemiology and clinical studies using human volunteer subjects. Wide ranges of pollutants known or suspected to cause health problems are studied. The research focuses on air pollutants, water pollutants, toxic substances, hazardous wastes, pesticides and non-ionizing radiation. The laboratory participates in the development and revision of air and water quality criteria and health assessment documents on pollutants for which regulatory actions are being considered. Direct support to the regulatory function of the Agency is provided in the form of expert testimony and preparation of affidavits as well as expert advice to the Administrator to assure the adequacy of environmental regulatory decisions involving the protection of the health and welfare of all U.S. inhabitants.

The purpose of this research program was to enable EPA scientists to correlate the results of the detailed chemical characterization with those from other research programs testing the potential biological activity (i.e., mutagenicity) of the concentrates.

F. Gordon Hueter, Ph.D.
Director
Health Effects Research Laboratory

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16. ABSTRACT

The goal of this research program was to provide a detailed chemical characterization of organic material concentrated from large volumes (1,500 liters to 15,000 liters) of finished drinking water (DW) and finished water from advanced waste treatment (AWT) plants. The approach used was organic compound identification based on glass capillary gas chromatography-mass spectrometry (GC-MS) analysis of the fractionated concentrate. The purpose of the research program was to enable EPA scientists to correlate the results of the detailed chemical characterization with those from other research programs testing the potential biological activity (i.e., mutagenicity) of the concentrates. Fifteen DW concentrates, sixteen AWT concentrates and five concentrate production method blanks were analyzed.

The cities represented by the DW samplings were Cincinnati, Miami, New Orleans, Ottumwa (Iowa), Philadelphia and Seattle. Most of the unrecovered organic portion and the extracted material not amenable to GC-MS analysis appeared to be humic substances. In the 15 DW concentrates, 1091 organic compounds were identified in a total of 2383 detection instances.

The AWT plans sampled were located at Escondido, Lake Tahoe, Orange County and Pomona (all in California), Dallas, and Washington, D.C. (Blue Plains site). In the 16 AWT concentrates, 991 organic compounds were identified in a total of 2097 detection instances.

17. KEY WORDS AND DOCUMENT ANALYSIS

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VOLUME 3
ABSTRACT

Volumes 1 and 2 of this report present analysis results of organic material concentrated from large volumes (1,500 to 15,000 liters) of drinking water (DW) and advanced waste treatment (AWT) plant water. As an ancillary task to that major focus of this research program, it was required to analyze numerous samples which represented smaller volumes (10 to 50 liters) of water. The function of these small-volume samples was to provide information relevant to assessing the performance of the reverse osmosis (RO) pre-concentration process used in the generation of the large-volume organic concentrates and also to provide information relevant to a comparison of the effectiveness of the analytical scheme employed in this research program to that of other analytical schemes of interest to the EPA using identical field samples.

In the approach to this problam, two key method development aspects were required: 1. The previously developed analytical scheme (see Volume 1) had to be sufficiently simplified to enable analysis of 4 small-volume samples with the same resource expenditure as one large-volume sample, 2. An ultra-clean technique for the extraction of 10-liter DW samples enabling detection of sample constituents present at less than 0.1 parts per billion (ppb) had to be demonstrated.

Four main groups of samples were analyzed. One group of 4 samples documented the adequacy of the performance capability of the 10-liter extraction procedure by analysis of two reagent water and two Cincinnati tap water (DW) 10-liter samples. One of the tap water samples was lyophilized, and the analysis results indicated that this method of concentration resulted in the loss of many volatile constituents and the addition of a number of artifact compounds. A second group of 18 samples were intended to provide information regarding RO pre-concentration performance on moderately contaminated DW (Jefferson Parrish, Louisiana) and pristine DW (Poplarville, Mississippi). However, artifacts introduced to these samples by the XAD-2 resin used to produced them made the data useful only as a detailed documentation of the chemical species present in XAD-2 resin bleed material. The third and fourth groups of 13 and 7 samples, respectively, were associated with sampling at the Cincinnati waterworks at points before and after treatment of the finished DW stream by granular activated carbon (GAC) contactors. Analysis of samples identical to these 20 by EPA using different methods provided comparative results that have been published. Analysis results of these 20 samples indicate that: 1. Many apolar organic species are not recovered by RO pre-concentration, 2. XAD-2 adsorption was more effective than RO in the recovery of apolar organic species, 3. Batch liquid-liquid extraction is superior to closed loop stripping for the preparation of samples when analysis of polar, ionizable or low volatility compounds is required but the latter method is considerably superior in both absolute performance and cost effectiveness when apolar, moderatly volatile compounds are of interest, 4. GAC treatment of DW was highly effective for the removal of most of the organic material present which was amenable to GC-MS analysis and 5. The GAC contactor which had been in use for 7 weeks was less effective at removing more polar organic materials than one in use for only 1 week.

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ABBREVIATIONS AND SYMBOLS

ABBREVIATIONS IN THE TEXT

AWT -- advanced waste treatment
BLLE -- batch liquid-liquid extraction
CA -- refers to cellulose acetate RO membrane
CLSA -- closed loop stripping analysis
DFTPP -- decafluorotriphenylphosphine
DW -- drinking water
FC-43 -- perfluorotributylamine
GAC -- granular activated carbon
GC -- gas chromatography or gas chromatographic
GC-MS -- gas chromatography-mass spectrometry
GSRI -- Gulf South Research Institute
HEB -- hexaethylbenzene
HERL -- Health Effects Research Laboratory
IS -- internal standard
KD -- Kuderna-Danish (distillation technique)
m/e -- mass to charge ratio
ng/l -- nanogram per liter, concentration
NYL -- refers to nylon RO membrane
%HEB -- Size of a GC peak expressed as a percentage of the internal standard peak, HEB.
RO -- reverse osmosis
RS -- relative size; a parameter assigned to all GC peaks for approximate quantification. See discussion in text and Volume 1
SP1000 -- a polar GC liquid phase consisting of Carbowax 20M (polyethylene glycol) terminated with nitroterephthalic acid
XAD-2 -- identifies a sample produced by adsorption/elution using XAD-2 resin (polystyrene/2% divinyl benzene copolymer, Rohm and Haas Co.)

ABBREVIATIONS IN THE COMPUTER-PRINTED TABLES

CAS NO. -- numbers with five or more digits: Chemical Abstracts Service compound registry number; numbers with four or fewer digits are Battelle numbers
COL. 1 -- refers to analysis on the SP1000 GC column
COL. 2 -- refers to analysis on the SP2100 GC column (not applicable in this volume)
CONC. -- concentration in the original water, in nanograms per liter
%HEB -- Size of a GC peak expressed as a percentage of the internal standard peak, HEB.
FRACTION 2 -- the methylated acid fraction

FRACTION 4 -- the neutral components left after removal of the extractable acids

FRACTION 9 -- the fraction from methylene chloride elution of silica gel

POS. OR TENT. ID -- identification mode; pertains to whether compound identifications are confirmed or tentative (see "P" and "T")

P -- designates a compound identification which was proved correct by analysis of a standard

RS -- relative size; a parameter reflecting the size of the GC peak for an identified compound; see discussion in text and Volume 1

T -- designates a compound identification which is tentative, i.e., it has not been proved correct by analysis of a standard

SYMBOLS USED IN THE COMPUTER-PRINTED TABLES

The following four symbols may appear to the left of the compound name:

* -- designates a compound on the list of 53 compounds (see Table 4, Volume 1)

+ -- designates a compound which is on EPA's Consent Decree Priority Pollutant list (semi-volatile compounds)

$ -- designates a compound which is on the Chemical Indicators of Industrial Pollution list (Federal Interim Primary Drinking Water Regulations, February 9, 1978)

% -- designates a compound which is an entry in the EMIC data base of compounds on which bioactivity data is available from Oak Ridge National Laboratory

SAMPLE CODE NAMES

Four-digit and three-digit code names are used throughout the text to refer to the 33 samples which are the subject of this volume. This code naming system is explained in detail in Appendix A. Sample code name meanings for the Cincinnati GAC contactor A samples can also be found in Figure 2 and Tables 3 and 4 while those for GAC contactor D can be found in Figure 3 and Tables 7 and 8.

BRIEF DESCRIPTION OF ALL VOLUMES OF THE FINAL REPORT

There are three volumes of this Final Report on EPA contract 68-03-2548. Each is briefly described below and the Tables of Contents of Volumes 1 and 3 are reproduced in Appendix B.

VOLUME 1

Volume 1 covers all aspects of analysis of the concentrates produced from large volumes (greater than 1415 liters (400 gallons)) of drinking water (DW) and advanced waste treatment (AWT) water. Eight key computer-printed tables which show organic compound identification results in integrated listings for the related sets of concentrates (DW and AWT) are contained in Volume 1. All discussion of the analysis results for large-volume DW and AWT concentrates as well as a complete description of the analytical scheme, computerized data management and accounting of all contract deliverables are contained in Volume 1.

VOLUME 2

Volume 2 contains 22 computer-printed tables which comprise the complete set of compound identification results covering the DW and AWT large-volume concentrates. Eight of these 22 tables are also incorporated in Volume 1 as the "core" set of information. The 14 computer-printed tables of Volume 2 which do not appear in Volume 1 provide the following additional information:

1. Identification status (confirmed or tentative) for all instances of compound identification in concentrates.
2. Systematic names, molecular formulas and molecular weights of all identified compounds.
3. Functional group information for each concentrate showing the total relative size values for each functional group on each of the two GC columns (SP1000 and SP2100).

VOLUME 3

Volume 3 covers the analysis of all small volume (10 to 30 liters) samples. These samples comprise the following sets:

1. A group of 13 samples of DW associated with granular activated carbon (GAC) contact treatment using unit "A" at the Cincinnati Waterworks.

2. A group of 7 samples, analogous to No. 1, above, associated with GAC contactor unit "D".
3. A group of 9 samples produced to monitor the reverse osmosis processing of DW sampled at Jefferson Parrish (New Orleans) Louisiana.
4. A group of 4 10-liter samples consisting of two reagent water blanks and two Cincinnati DW samples of which one was processed by lyophylization.

All of the compound identifications results for the above four sets of samples are presented and discussed in Volume 3. In addition, the modified analytical scheme used for these samples is presented in detail and compared to that used for the large-volume samples (Volume 1).

ACKNOWLEDGMENTS

Through the course of this three-year research program, many members of Battelle's technical staff have made significant contributions to the high quality of the results that were obtained. Denis C.K. Lin deserves special recognition for his major contribution to the conceptualization and development of the analytical scheme, results report format and computerized management of the extremely large database. His incorporation of glass capillary GC columns and a large number of deuterated internal standards were definitely "state of the art" at that time (1977). Other Battelle scientists and their contributions to this work include:

Laurence E. Slivon--Design and validation of the computer search and quantification capability; System/150 to INCOS data transfer; EPA/NIH/NSRDS library search implementation; high-density 9-track taping of GC-MS data; numberous utility programs for System/150; mass spectral data interpretation

Bruce A. Petersen--Analytical scheme design, quality control development, and mass spectral data interpretation

Roderick G. Warren--Implementation of the NUCLEUS data management and report production systems

Roger L. Foltz and Richard M. Thompson--Mass spectral data interpretation

Susan G. Watson--Confirmation of compound identification and mass spectral data interpretation

Timothy L. Hayes--GC-MS data processing, 10-liter extraction, data acquisition

Vanessa R. Goff--GC-MS data acquisition, quality control, and mass spectral data interpretation

Denise A. Contos--Concentrate partitioning, residue weight determinations, standards preparation, sample analysis tracking, and GC-MS data searching and quantification

Daniel G. Aichele--NUCLEUS system interaction and operation, report generation and coordination

Patricia P. Kelley--Report system development and production, NUCLEUS interaction

Joseph P. Tabor--GC-MS data screening for artifacts

Cynthia A. Schweiger and Bruce E. Urbschat--Assistance with NUCLEUS operations

The author, as senior team member in the early stages and principal investigator since 1979, was involved in all of the above cited activities except the development of System/150 operation programs.

SECTION 1

INTRODUCTION

STATEMENT OF THE PROBLEM

In Volume 1 of this report are presented the results of glass capillary gas chromatography-mass spectrometry (GC-MS) analysis of organic concentrates prepared from large volumes (1,500 to 15,000 liters) of drinking water (DW) and advanced waste treatment (AWT) water. The method used to prepare these concentrates was based on pre-concentration using reverse osmosis (RO). Evaluation of the effectiveness of RO pre-concentration was an ancillary task of this research program. In conjunction with the task of evaluating the effectiveness of the RO pre-concentration processing an opportunity was realized to perform some of the sampling in such a way that the results would be useful for other research programs in progress at the EPA Health Effects Research Laboratory (HERL).

The additional HERL research goal was concerned with water treatment by contact with granular activated carbon (GAC) which shows much promise for the removal from DW of many organic species present at trace levels--especially those resulting from industrial pollution. The method is currently in wide use in Europe. This research goal is one aspect of HERL's primary responsibility. The set of samples for which this multiplicity of purposes was realized were associated with an investigation of the effectiveness of GAC contactors at the Cincinnati, Ohio, waterworks. The samplings associated with Cincinnati waterworks GAC units were performed to enable comparison of four different GC-MS based methods of analysis: 1. EPA Method 624 volatile analysis, 2. Grob closed loop stripping analysis (CLSA) using 1-liter samples, 3. XAD-2 adsorption/diethyl ether elution using 10-liter samples, and 4. Batch liquid-liquid extraction using 10-liter samples.

Two other sets of samples were associated with: (a) monitoring the RO pre-concentration performance for DW sampling at Jefferson Parrish (New Orleans), Louisiana, and Poplarville, Mississippi; and (b) validating a 10-liter liquid-liquid extraction procedure for use on the Cincinnati samples.

Results of analysis of the large-volume concentrates (Volume 1) showed that a multitude of organic compounds can be detected in many finished DW supplies but that most compounds are present at the trace (sub-part per billion, ppb) level. A major constraint on the approach to the problem was that the task of monitoring the performance of the RO concentrator required that a relatively large number of samples would have to be analyzed. In addition, the samples represented a far smaller volume of water (i.e., 10 liters compared to 1500 liters) and, thus, would be far less complex than the large volume concentrates with which Project 68-03-2548 was originally concerned. For this reason, development of a new analytical scheme was required to enable a cost-effective analysis of this greater number of relatively clean samples without an increase in the required resources.

APPROACH TO THE PROBLEM

The approach to the analytical problem required optimization of two key aspects: 1. because the samples contained very low levels of organic material, processing of sample volumes of about 10 liters with the lowest possible level of artifact introduction was necessary, and 2. the larger number of samples required scaling down the original, large-volume concentrate analysis scheme (Volume 1) to allow processing of four small-volume samples at the same cost as one of the large-volume concentrates. Two approaches to the requirement of a multi-liter sample size were taken. In one, the contractor responsible for preparation of the large-volume concentrates (Gulf South Research Institute, GSRI) extracted samples taken from the RO apparatus at various stages using XAD-2 resin extraction/diethyl ether elution. In the second approach, similar samplings representing 10 liters of original water were taken at various stages of the RO processing procedure as well as points before and after FAC contactor treatment. These samples were processed by a 10-liter batch liquid-liquid employing ultra-clean methodology. Duplicate samples were taken at selected points for concentration by XAD-2 adsorption/diethyl ether elution. All of these samplings are described in Section 4.

The approach to the second key aspect required modification of the analytical scheme for large-volume concentrates to allow analysis of four samples using the same commitment of project resources as that required for one large-volume concentrate) is detailed in Section 5, Analytical Scheme.

SECTION 2

CONCLUSIONS

There are five principal conclusions which can be based on the results of the research reported here:

1. It is possible to successfully identify organic pollutants in water samples as pure as finished drinking water (DW) at concentrations below the 0.1 ppb (μg/l) level using a 10-liter sample and the special refinements of the bottle-stirbar liquid-liquid extraction described here. The critical aspects are: (a) use of freshly distilled extraction solvent, (b) exposure of sample to glassware heated to 450°C in a muffle furance, (c) heating of all glassware and sodium sulfate at 450°C for 8 hours immediately before use and (d) careful protection of the distilled extraction solvent, sample and all glassware from the laboratory environment.

2. Apolar trace level organic pollutants are more effectively recovered from water by XAD-2 resin than by reverse osmosis (RO) while the opposite is true for highly polar, ionizable and/or macromolecular materials.

3. Use of XAD-2 resin for extraction of trace level organic pollutants from DW requires extreme care in prior preparation of the resin with regard to removing extractable artifact materials.

4. Contact of DW with granular activated carbon (GAC) as a final waterworks treatment step was highly effective for the removal of essentially all organic constituents amenable to GC-MS analysis.

5. A GAC contactor unit which had been in use for 7 weeks was apparently less effective at removing organic contaminants than a similar unit which had been in service only one week. In agreement with expectations, highly polar and/or ionizable substances were the first materials to break through the GAC contactor unit as its capacity declined with use.

SECTION 3

RECOMMENDATIONS

In Volume 1, the minor recommendations made regarding possible improvements to the analytical scheme apply to the analytical scheme used for the small volume samples reported here, and they will not be repeated. The analysis results show that the 10-liter extraction procedure is well optimized although some further refinement would undoubtedly be achieved upon further use of the procedure.

In contrast, the data strongly suggest that the use of reverse osmosis (RO) for organic compound pre-concentration has some demonstrable deficiencies with regard to recovery of high interest apolar substances. The series of experiments designed to test this RO performance criteria were well designed to monitor apolar material recovery through the various stages of the RO processing apparatus since XAD-2 resin adsorption/diethyl ether elution is optimal for recovery of these same apolar species. Unfortunately, the use of XAD-2 resin for this purpose has extremely exacting requirements with regard to prior resin cleanup and storage and handling before use, and this evaluation effort failed because of excessive levels of resin artifact materials. While there are numerous reportedly successful protocols for the use of XAD-2 resin none are highly reliable for the analyst less experienced in using XAD-2 resin in such highly critical applications as these. Since it is not chemically reasonable that all of the artifact material could not be stripped from XAD-2 resin, some definitive further work in this area would provide a valuable service to other trace-level water analysts and also provide cost-effective methodology for assessing the performance of RO pre-concentration under actual field sampling conditions. Although the 10-liter extraction procedure is less cost-effective than a reliably artifact-free XAD-2 adsorption/diethyl ether elution approach, the former is, indeed, presently capable of providing the basis for analyses to monitor the effectiveness of RO pre-concentration. HERL-CI currently is managing extramural research programs to characterize and validate a number of large-volume organic concentrate production methods including RO and adsorption/elution based approaches. Use of the 10-liter ultraclean liquid-liquid extraction procedure for validation of recovery performance methods now under development would provide critical, independent performance evaluation of these methods at the optimal point in time.

SECTION 4

DESCRIPTION OF THE SAMPLES

There are four distinct group of samples for which the results of each are discussed in Section 6, Results and Discussion. These four groups are:

1. Thirteen samples associated with GAC contactor A at the Cincinnati waterworks
2. Seven samples associated with GAC contactor D at the Cincinnati waterworks
3. Four samples associated with method validation of the 10-liter extraction procedure described in Section 5
4. Nine samples associated with DW RO processing at New Orleans and nine similar samples from Poplarville, Mississippi.

Some or all of the samples of groups 1, 2 and 4, above, were taken from various points of the RO pre-concentration processing performed by GSRI. The details of the RO pre-concentration apparatus and procedure have been previously described (3); a schematic diagram of the RO unit is shown in Figure 1. Each of the four sets of samples listed above are described in detail below.

CINCINNATI GAC CONTACTOR A SAMPLES

The schematic flow diagram in Figure 2 shows the sampling points with respect to water treatment with GAC contactor unit A and various stages of the RO processing on January 14, 1980. The four-digit sample identification codes appear inside the oval enclosures of Figure 2 which designate the 13 analyzed samples. The 4-digit sample code is the second through the fifth digits of the 6-digit GC-MS file naming system for the small volume samples which is explained in Appendix A. Note that the first two digits of the 4-digit code are "T4" which characterize these samples as the fourth Cincinnati sampling. In subsequent discussions, this set is referred to as the T4 or GAC contactor A samples. All of these samples except 6 represent 10 liters of sampled volume. The volumes corresponding to the 6 samples which represent water after some degree of RO processing are: 10-fold brine, 12 liters, samples T4R1 and T4R4; 100-fold brine, 16 liters, samples T4R2 and T4R5; and 200-fold brine, 32 liters, samples T4R6 and T4G2. The accuracy of the brine concentration factor (and, therefore, also of the volume represented) was estimated at 10 percent. The RO processing was performed at the Cincinnati waterworks by GSRI personnel. The samplings not associated with RO processing

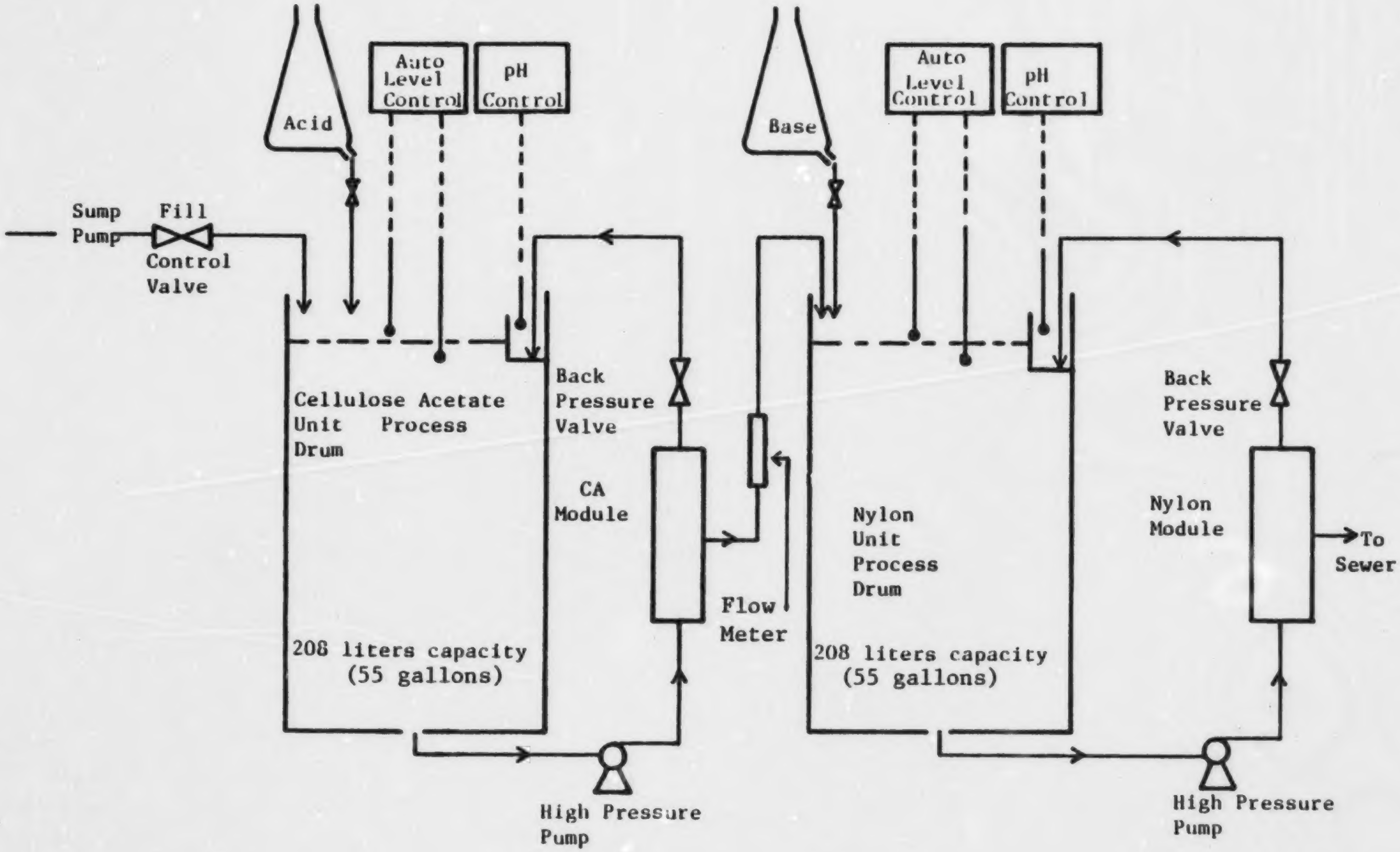
Acid
Auto Level Control
pH Control
Base
Auto Level Control
pH Control
Sump Pump
Fill Control Valve
Cellulose Acetate Unit Process Drum
Back Pressure Valve
CA Module
208 liters capacity (55 gallons)
Flow Meter
Nylon Unit Process Drum
208 liters capacity (55 gallons)
Back Pressure Valve
Nylon Module
To Sewer
High Pressure Pump
High Pressure Pump

Figure 1. Schematic diagram of the reverse osmosis concentrator used by GSRI. (Taken from EPA publication 600/2-78-016, February, 1978; available through NTIS)

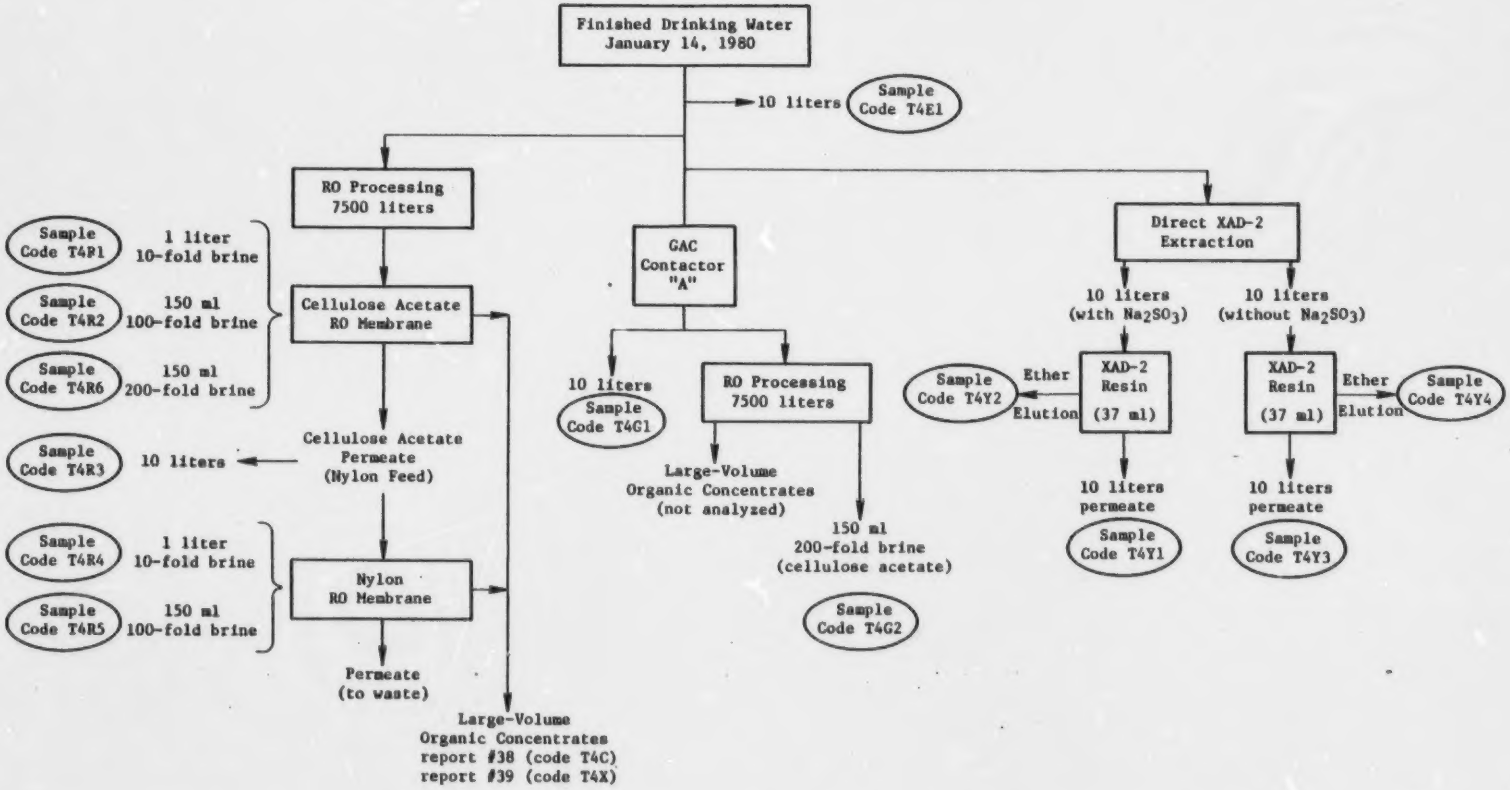
Finished Drinking Water
January 14, 1980
10 liters
Sample Code T4E1
RO Processing 7500 liters
Cellulose Acetate RO Membrane
Sample Code T4P1
1 liter 10-fold brine
Sample Code T4R2
150 ml 100-fold brine
Sample Code T4R6
150 ml 200-fold brine
Cellulose Acetate Permeate (Nylon Feed)
Sample Code T4R3
10 liters
Nylon RO Membrane
Sample Code T4R4
1 liter 10-fold brine
Sample Code T4R5
150 ml 100-fold brine
Permeate (to waste)
Large-Volume Organic Concentrates report #38 (code T4C) report #39 (code T4X)
GAC Contactor "A"
10 liters
Sample Code T4G1
RO Processing 7500 liters
Large-Volume Organic Concentrates (not analyzed)
150 ml 200-fold brine (cellulose acetate)
Sample Code T4G2
Direct XAD-2 Extraction
10 liters (with Na_2SO_3)
10 liters (without Na_2SO_3)
XAD-2 Resin (37 ml)
Ether Elution
Sample Code T4Y2
10 liters permeate
Sample Code T4Y1
XAD-2 Resin (37 ml)
Ether Elution
Sample Code T4Y4
10 liters permeate
Sample Code T4Y3

Figure 2. Sampling flow diagram for the Cincinnati GAC contactor A samples.

and the XAD-2 adsorption/diethyl ether elution procedure indicated in Figure 2 were performed by HERL personnel. Samples corresponding to pre- and post-GAC contactor A and pre- and post-XAD-2 adsorption were analyzed by HERL using Grob CLSA and EPA Method 624. The results of those analyses have been compared with those presented here, and that comparison is the subject of reference 4.

CINCINNATI GAC CONTACTOR D SAMPLES

The schematic flow diagram in Figure 3 shows sampling points for the 7 samples associated with Cincinnati GAC contactor D on January 28, 1980, in exactly analogous fashion to those cited above for GAC contactor A. Note that the 7 samples shown in Figure 3 have 4-digit code names beginning "T5" (see above discussion of the 4- and 6-digit code system). In subsequent discussions, these samples are referred to as the T5 or GAC contactor D samples. As for the T4 samples, GSRI performed the RO pre-concentration at the Cincinnati waterworks, and the samplings not associated with RO processing were performed by HERL personnel. HERL also performed Grob CLSA and EPA Method 624 analysis on samples analogous to the T5 set, and the comparison of HERL's analysis results with those presented here for the T5 samples can be found in reference 4.

SAMPLES FOR MONITORING RO PRE-CONCENTRATION OF DW AT JEFFERSON PARRISH, LOUISIANA, AND POPLARVILLE, MISSISSIPPI

Four samplings points are relevant to monitoring the RO apparatus shown schematically in Figure 1:

1. The starting water, designated cellulose acetate RO feed
2. The brine concentrate produced by the cellulose acetate RO unit
3. The cellulose acetate RO permeate designated nylon RO feed
4. The concentrate produced by the nylon RO unit.

The fifth sampling point, nylon RO permeate, was not considered by HERL to be significant enough for analytical evaluation.

For ideal RO pre-concentration performance, all of the chemical species identified in sample No. 1 should be found in sample Nos. 2, 3 and 4; and sample Nos. 2, 3 and 4 should not contain any species not found in sample No. 1. To obtain the necessary samples, GSRI processed aliquots by direct XAD-2 adsorption/diethyl ether elution. These aliquots were taken from full-scale RO processing of DW sampled at the Jefferson Parrish, Louisiana, waterworks on January 5 and 6, 1979 and at the Poplarville, Mississippi, waterworks on March 2, 1979. The same method, described below, was used to generate samples for the above four catagories at both acidic and basic pH (8 samples) plus one XAD-2 blank elution for both sites.

Fifty-liter aliquots of cellulose acetate RO feed water and nylon RO feed water were acidified to pH 2 and passed through separate XAD-2 resin columns. The columns were eluted with diethyl ether with subsequent sample concentration

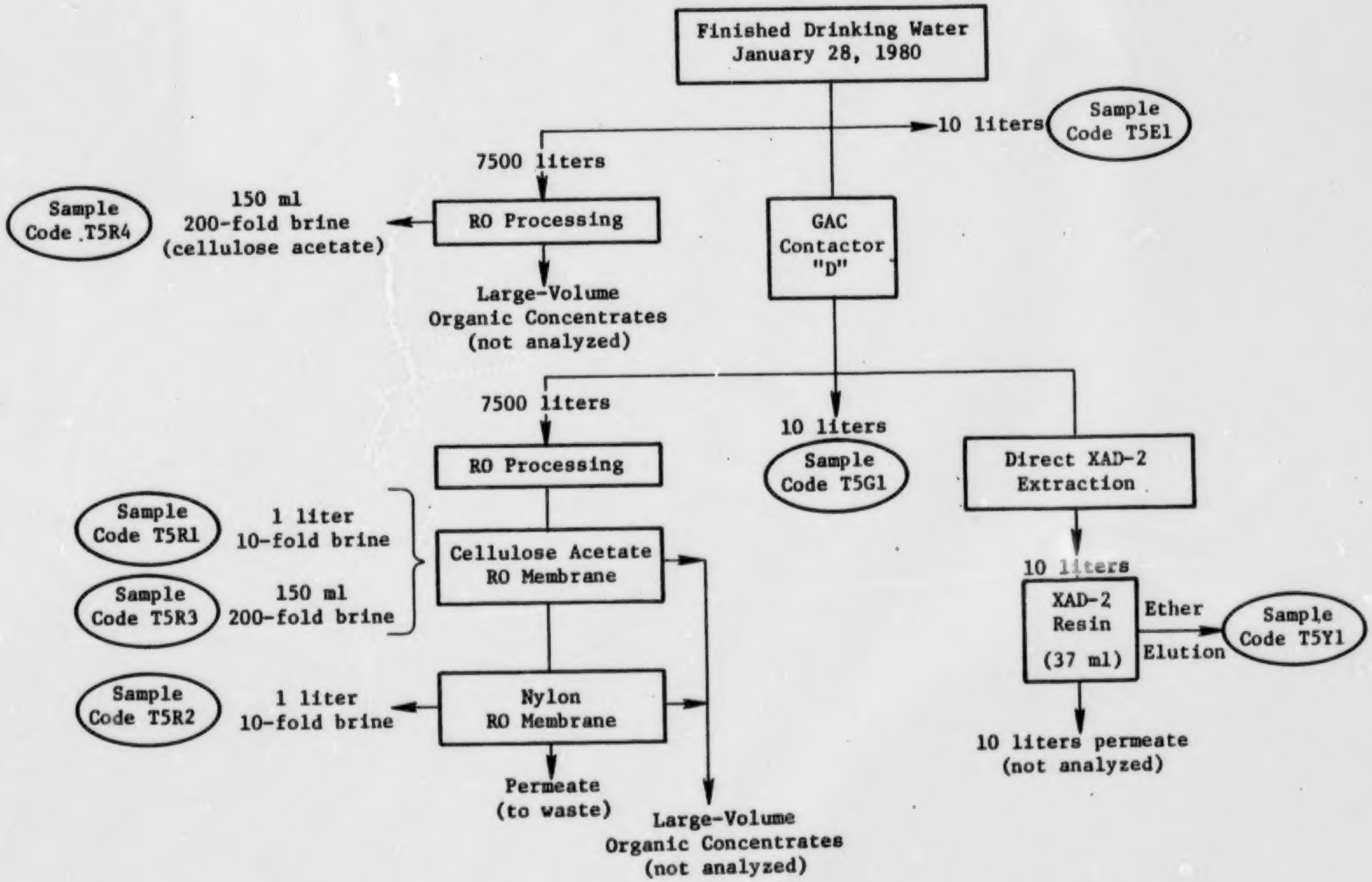
Finished Drinking Water
January 28, 1980
10 liters
Sample Code T5E1
7500 liters
RO Processing
150 ml
200-fold brine
(cellulose acetate)
Sample Code T5R4
Large-Volume
Organic Concentrates
(not analyzed)
GAC Contactor "D"
7500 liters
RO Processing
10 liters
Sample Code T5G1
Direct XAD-2 Extraction
Sample Code T5R1
1 liter
10-fold brine
Cellulose Acetate RO Membrane
Sample Code T5R3
150 ml
200-fold brine
10 liters
XAD-2 Resin (37 ml)
Ether Elution
Sample Code T5Y1
Sample Code T5R2
1 liter
10-fold brine
Nylon RO Membrane
10 liters permeate
(not analyzed)
Permeate
(to waste)
Large-Volume
Organic Concentrates
(not analyzed)

Figure 3. Sampling flow diagram for the Cincinnati GAC contactor D samples.

by solvent evaporation to 15 ml or less. The RO units were operated until a 10-fold brine concentration factor was achieved and 5-liter aliquots of the cellulose acetate and nylon brines (each corresponding to 50 liters of original water) were acidified and concentrated on XAD-2 resin as described above. A pH 10 sample was also prepared corresponding to each of the four pH 2 samples described above. A ninth sample corresponding to a blank elution of the XAD-2 resin used for each set of samples was also prepared.

SAMPLES FOR METHOD VALIDATION OF THE 10-LITER EXTRACTION PROCEDURE

HERL provided four 10-liter samples for use in validating the 10-liter liquid-liquid extraction procedure (see Section 5) used for the Cincinnati GAC contactor A and D sets of samples. Two of these samples were reagent water (designated Super-Q water) which was specially purified at the HERL laboratories by a procedure described in Section 5. The other two samples corresponded to 10 liters of Cincinnati tap water sampled at the HERL laboratory. One of these samples was concentrated by lyophylization and then reconstituted to the original 10-liter volume with Super-Q reagent water.

SECTION 5

ANALYTICAL SCHEME

RATIONALE FOR THE ANALYTICAL SCHEME

The first task of Project 68-03-2548 was to develop an analytical scheme to provide optimal organic compound identification results for extremely complex organic concentrates generated from RO processing of very large volumes (1,500 to 15,000 liters) of water. That analytical scheme is presented in detail in Volume 1 of this report. The objective to analyze small-volume samples (for example, 10 liters) which would enable an assessment of the effectiveness of the RO processing used for concentrate production required further development work in two areas:

1. Development of an ultra-clean batch liquid-liquid extraction of 10-liter samples which would be sufficiently free of artifacts to enable reliable detection of sample components present at the sub-part per billion level

2. Modification of the original concentrate analytical scheme to allow the analysis of four of these small-volume samples with the same resource expenditure as required for one large-volume concentrate.

The latter requirement, above, necessitated some revision in scope as compared to the former scheme. The modified scheme is presented in detail below. Briefly, the principal differences between the small-volume analytical scheme and the previously developed scheme can be summarized as follows:

Additions to the previous scheme:

1. Efficient distillation of extraction solvent

2. Development of an ultra-clean 10-liter extraction scheme

3. Expression of all GC-MS peak heights as a percent of the internal standard, hexaethylbenzene (HEB), and modification of the data management software to display this parameter in computer-generated listings

Deletions from the previous scheme:

1. Samples were analyzed only on one GC column (SP1000)
2. Bases were not extracted
3. GC-MS analysis of two fractions instead of four: derivatized acids and neutral compounds
4. GC-MS data were not searched for the list of 54 specific search compounds
5. No response factor-based quantification was performed
6. No attempt was made to purchase compounds for identification confirmation which had not been previously identified
7. Reports of analysis results were not prepared separately from the project final report.

Important features which were retained:

1. All quality control measures
2. Comprehensive main-frame computer management of identification results and data processing for report generation
3. Use of thirteen deuterated internal standards (two of which are bases and, therefore, not recovered)
4. Manual checking of all mass spectral library matching results and manual interpretation as necessary
5. Attempted confirmation of all identifications using the existing confirmation data base.

DISTILLATION OF EXTRACTION SOLVENT

Approximately 4.2-liter batches of Burdick and Jackson "Distilled in Glass" methylene chloride (all of the same lot number) were redistilled in a 5-liter flask equipped with a vertical 60 cm x 1.8 cm ID column packed with medium size glass helices. The receiver was the original one gallon solvent bottle which was tightly sealed to the vented condenser delivery adapter using three teflon washers. The condenser adapter was vented to the atmosphere through a 100 ml cartridge of granular activated charcoal to prevent exposure to organic material in the laboratory air. A slight positive pressure (about 2 mm of water) of ultra high purity nitrogen (Matheson, 99.999%) was maintained throughout the distillation using a bubbler chamber. Additionally, the distillation pot/condenser and the receiving bottle were separately flushed with nitrogen before start up of each batch. Methylene chloride was distilled at a rate of 1.4 to 1.8 ml/min. The first 300 ml of distillate and the last 300 ml remaining in the pot were discarded. After distillation, methylene chloride was stored under nitrogen and used for extraction within three days.

REAGENT WATER

Organic-free reagent water (designated "Super-Q" water) was supplied by HERL-CI in cleaned (muffle oven; 450°C) one-gallon glass jugs filled without headspace and sealed with Teflon-lined screw caps. HERL-CI produced this water using a modified Milli-Q apparatus (Millipore) in which the ion-exchange cartridges of the Milli-Q system were replaced with activated carbon cartridges. The feed water was distilled at EPA. In addition, the system was operated strictly in a batch mode with careful flushing and disinfection after use to prevent microbial contamination.

LIQUID-LIQUID EXTRACTION OF 10-LITER SAMPLES

Two types of water samples were extracted: (1) samples which had not been partially concentrated by RO and (2) samples which had been concentrated 10 to 200-fold by RO (See Figures 2 and 3).

Preparation for Extraction

Samples which had not been pre-concentrated by RO were collected in one-gallon glass jugs heated in a muffle oven (450°C) with Teflon-lined screw caps by HERL personnel. Three one-gallon jugs filled without headspace were required for each 10-liter sample. A small amount of water (30 to 50 ml) was removed from each jug and the contents thoroughly mixed by shaking. Water was again removed by aspiration until 3.33 liters remained. This removal was accomplished by one of two methods. For jugs with known tare weights, a 5 kg capacity balance was used and water was removed to give a net weight of 3.33 kg. If the jug tare weight was unknown, another jug with exactly the same manufacturer mold markings was filled with 3.33 liters of water and sample water was removed to a level matching the reference jug.

Samples which had been partially concentrated by RO were collected in 1-liter (1.2-liter without headspace) Teflon-lined screw cap bottles (10-fold concentration factor) or 150 ml serum bottles (160-ml capacity without headspace) with Teflon-lined crimp caps (100-fold and 200-fold concentration factor). In order to ensure exact equivalence (with respect to sample extraction) between the 10-liter samples and the partially concentrated samples, the 1-liter and 150-ml samples were diluted to 10 liters with "Super-Q" reagent water (described above) before extraction. To prepare a partially concentrated sample for extraction, three 1-gallon jugs of reagent water were adjusted to a volume such that, after addition of one third of the partially concentrated sample, the final volume would be 3.33 liters. The partially concentrated sample was then poured directly into the three reagent water jugs, approximately by thirds, and mixed thoroughly with back-rinsing of the original sample bottle into one of the 3.33-liter samples. Finally, the exact volume of the partially concentrated sample was determined by filling the original container and decanting into a graduated cylinder.

Addition of Internal Standards

The deuterated internal standards listed in Table 1 were added to the water sample at the 0.6 ppb level (6 μg of each per 10 liters of sample). Each 3.33-liter portion received 33 μl of an 80 percent methanol solution which was added by syringe injection into the rapidly stirred sample.

Acidification of the Sample

Approximately 1.3 ml of concentrated H_2SO_4 was added drop wise to the rapidly stirring sample to increase the acidity to pH 2, as measured with narrow range pH paper.

Bottle-Stirbar Extraction

Each of the three 3.33-liter sample aliquots was extracted three times with re-distilled methylene chloride (250 ml, 100 ml and 100 ml). Each extraction was stirred for 40 min at the maximum stable speed with a 3-inch teflon-coated magnetic stirring bar which was stored under re-distilled methylene chloride between uses and rinsed with re-distilled methylene chloride just prior to use. The stirring was sufficient to bring the vortex within 5 cm of the jug bottom and resulted in a very fine and even solvent dispersion throughout the sample.

Removal and Concentration of the Extract

After stirring, the methylene chloride layer was allowed to settle completely. It was then withdrawn from the bottom of the tilted jug by suction into a 100 ml glass vessel for transfer to a drying column. All nine methylene chloride extracts of the three 3.33-liter aliquots were passed through a column of anhydrous Na_2SO_4 (twice heated in a muffle furnace at 450°C for 10 hours, about 50 gm in a 2 cm ID column with a glass frit bottom). The Na_2SO_4 drying column was rinsed with two 50 ml aliquots of re-distilled methylene chloride before use. The drying column and 1-liter receiving flask was assembled as a closed system. No final rinse of the drying column was employed.

The first extraction of the three 3.33-liter sample aliquots resulted in about 600 ml of methylene chloride, and the second and third extractions, together, yielded another 600 ml. The volumes of these two portions were simultaneously reduced by Kuderna-Danish (K-D) distillation using three ball columns, a 500 ml reservoir, and 25 ml bottom tubes. When either of these two volumes were reduced to the level of the bottom tube of the K-D

TABLE 1. DEUTERIUM-LABELED COMPOUNDS USED AS INTERNAL STANDARDS

Compound	Fractions in Which Compound is Recovered[a, b]
Pyridine-D_5	Not recovered
Aniline-D_5	Not recovered
Benzoic acid-D_5	Derivatized Acids
Phenol-D_5	Derivatized Acids
Eicosane-D_{42}	Aliphatic Hydrocarbons[c]
Bromobenzene-D_5	Aromatic/Medium Polarity
1,4-Dibromobenzene-D_4	" "
Naphthalene-D_8	" "
Chrysene-D_{12}	" "
Perylene-D_{12}	" "
Nitrobenzene-D_5	" "
Nitronaphthalene-D_7	" "
Dimethylterephthalate-D_4	High Polarity[c]

a) See Figure 4 for production details of the analyzed fractions.

b) Samples for which neutrals were not fractionated on silica gel contained all of the internal standards except pyridine-D_5, aniline-D_5, benzoic acid-D_5 and phenol-D_5 in the unpartitioned neutrals.

c) This fraction is not analyzed by GC-MS.

apparatus, the other extraction aliquot was added to it and distillation was continued to about 15 ml. The three-chamber condenser and 500-ml reservoir were then replaced with a modified micro Snyder distillation column, and the volume reduction was continued to about 4 ml. The sample was then transferred, with a 1.0 ml extraction solvent rinse, to a graduated 13 ml tube with a glass stopper for storage at -10°C.

General Precautions Employed to Avoid Contamination

- All glassware and anhydrous Na_2SO_4 were heated in a muffle furnace overnight at 450°C the evening preceding an extraction
- Glassware was removed from the muffle furnace while still warm (50 to 100°C) and immediately assembled with leak-tight closures
- Solvent distillation, extraction, and concentration were performed in a laboratory reserved strictly for this work
- All transfers, including those with disposable pipets, were accomplished with devices fitted with only glass and teflon parts. No rubber or plastic parts were used for any purpose where exposure to the sample was possible
- Re-distilled methylene chloride was periodically checked for adequate purity by K-D distillation of 500 ml aliquots, concentration to a final volume of 100 μl, addition of internal standard (2 μg), and analysis by glass capillary GC-FID or GC-MS as required.

EXTRACTION OF BLANKS

A simultaneous and parallel blank was extracted and concentrated each time 10-liter samples were processed. The blank consisted of one 3.33-liter sample of reagent water and was pH adjusted, fortified with deuterated internal standards, extracted, and concentrated exactly as described above except that K-D concentration was continued to a volume of 0.5 to 1.0 ml. Hexaethylbenzene (HEB) internal standard, 0.66 μg, was added to the sample in the K-D tube bottom and the sample was transferred after mixing but without rinsing, to a 3.0 ml Chromaflex (Kontes) graduated tube. Within 48 hours the blank extract was concentrated to 75 to 125 μl by the nitrogen blow-down technique described in a following section, and the blank concentrate was analyzed by glass capillary GC-MS within 3 hours of final volume reduction.

XAD-2 RESIN EXTRACTION OF SAMPLES

Of the Cincinnati samplings shown in the flow diagrams in Figures 2 and 3, three concentrate samples were generated by XAD-2 resin adsorption/diethyl ether elution. Two of these were associated with GAC contactor "A" and the third was associated with GAC contactor "D". These XAD-2 generated concentrates were produced by EPA at HERL-CI. A detailed description of the experimental procedure, based on the method described by Junk, et al., (2) has been reported (4). A brief outline of this procedure is presented below. is presented below.

1. XAD-2 resin was cleaned by successive 24 hour soxhlet extractions using methanol, acetonitrile, ethyl ether, and methanol
2. The resin was exchanged into reagent water (four times) and packed into 2.7 cm diameter by 6.5 cm columns (37 cc) with silanized glass wool plugs at the inlet and outlet
3. The resin column was washed with 1 liter of reagent water before the 10-liter sample (adjusted to pH 2) was passed through the column at a flow of about 28 ml/min
4. The XAD-2 column was eluted with 3 bed-volumes of freshly distilled diethyl ether which was then dried with anhydrous Na_2SO_4 and evaporated to about 1 ml by K-D distillation

The XAD-2 concentration approach used by GSRI for the sampling at Jefferson Parrish, Louisiana, and Poplarville, Mississippi, for RO monitoring purposes was briefly outlined in Section 4; further details are available from HERL-CI.

SAMPLE PARTITIONING

Aliquot for Unpartitioned Analysis

Sample extract concentrates from the 10-liter extraction and the HERL-CI and GSRI supplied XAD-2 diethyl ether eluates were diluted to 5.0 ml with redistilled methylene chloride. Ten percent of the diluted sample (500 µl) was removed for unpartitioned GC-MS analysis and stored in a 3.0 ml Chromaflex tube at -10°C. Immediately before GC-MS analysis, this volume was reduced under nitrogen to 30 to 50 µl and 0.2 µg of internal standard (HEB) was added. The remaining 90 percent of the diluted sample was fractionated into a derivatized acid fraction and one of two types of neutral fractions. Preparation procedures for the analysis of these fractions are described below and shown schematically in Figure 4.

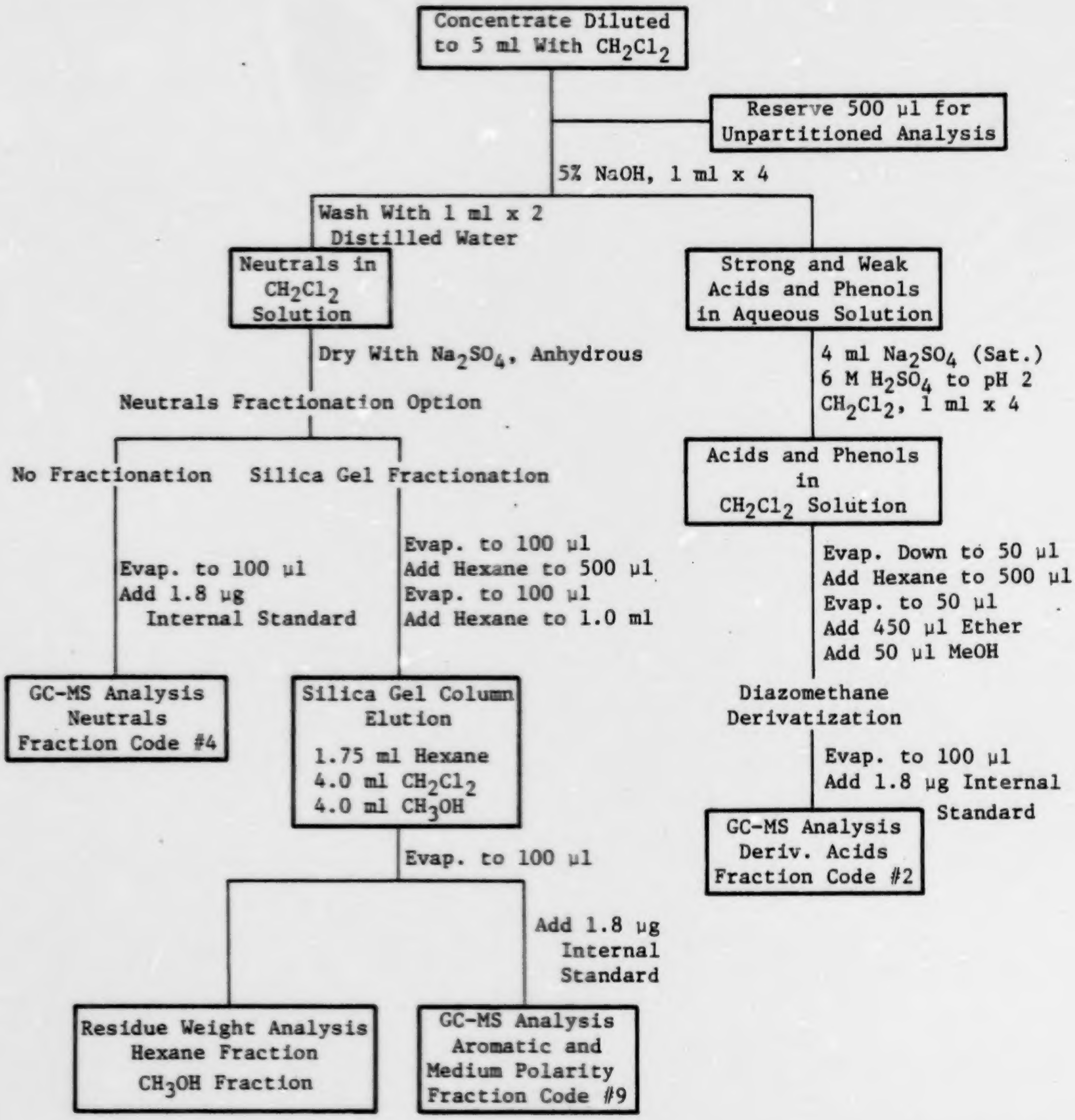
Concentrate Diluted to 5 ml With CH_2Cl_2
Reserve 500 µl for Unpartitioned Analysis
5% NaOH, 1 ml x 4
Wash With 1 ml x 2 Distilled Water
Neutrals in CH_2Cl_2 Solution
Strong and Weak Acids and Phenols in Aqueous Solution
Dry With Na_2SO_4, Anhydrous
Neutrals Fractionation Option
No Fractionation
Silica Gel Fractionation
4 ml Na_2SO_4 (Sat.)
6 M H_2SO_4 to pH 2
CH_2Cl_2, 1 ml x 4
Acids and Phenols in CH_2Cl_2 Solution
Evap. to 100 µl
Add 1.8 µg Internal Standard
Evap. to 100 µl
Add Hexane to 500 µl
Evap. to 100 µl
Add Hexane to 1.0 ml
Evap. Down to 50 µl
Add Hexane to 500 µl
Evap. to 50 µl
Add 450 µl Ether
Add 50 µl MeOH
GC-MS Analysis Neutrals Fraction Code #4
Silica Gel Column Elution
1.75 ml Hexane
4.0 ml CH_2Cl_2
4.0 ml CH_3OH
Diazomethane Derivatization
Evap. to 100 µl
Add 1.8 µg Internal Standard
GC-MS Analysis Deriv. Acids Fraction Code #2
Evap. to 100 µl
Add 1.8 µg Internal Standard
Residue Weight Analysis Hexane Fraction CH_3OH Fraction
GC-MS Analysis Aromatic and Medium Polarity Fraction Code #9

Figure 4. Sample extract fractionation scheme.

Derivatized Acid Fraction

The 4.5 ml methylene chloride solution remaining after removal of the portion for unpartitioned analysis was agitated for 1.0 min with 1.0 ml of 40 percent NaOH solution to remove the ionizable acids into the aqueous phase. After low speed centrifugation, the aqueous phase was removed, using a disposable pasteur pipet equipped with a teflon sealed gas-tight syringe operator, and placed in a 10 ml separatory funnel. This extraction was performed four times. Saturated Na_2SO_4 (4 ml) was added to the extracted acids to effect a salting out of the back extraction. The aqueous phase was acidified with 12 N H_2SO_4 (pH 2, using narrow range paper) and the acids were back-extracted four times (1 min shake-out) with 1 ml aliquots of re-distilled methylene chloride. The volume of the extracted acids was reduced by evaporation using a very slow flow of nitrogen in a 3.0 ml Chromaflex tube to about 100 µl; 500 µl of hexane was added and the volume was again reduced by evaporation to about 50 µl. After addition of 50 µl of methanol and 450 µl of diethyl ether, the acids were methylated with diazomethane bubbled into the sample from a gas-train generator. The methylation reaction was allowed to proceed for about 5 min. The reaction was then stopped by final volume reduction (as above) to 100 to 150 µl at which time 1.8 µg of HEB internal standard was added.

After removal of the acids, above, the remaining neutrals in methylene chloride solution were washed twice with distilled water to remove any NaOH residue and dried with 500 to 700 mg of granular anhydrous Na_2SO_4 which had been heated to 450°C in a muffle furnace.

Neutral Fraction

Fractionation on silica gel, used very successfully to produce aliphatic, aromatic, medium polarity, and high polarity fractions for the large-volume samples, was simplified to produce the neutral fractions for the small-volume samples. The simplification was obtained by combining the aromatic and medium polarity fractions in a single elution (this fraction was the only one to be analyzed by GC-MS). The aliphatic and high polarity fractions were eluted from the silica gel column but used only for residue weight analysis. This neutral fractionation scheme, shown in Figure 4, worked well but proved to be unnecessary for the cleanest DW samples. Thus, for some samples, the unpartitioned neutral fraction was analyzed directly.

Direct Analysis of the Neutrals. Nine samples were analyzed directly for neutral compounds (i.e., without silica gel fractionation):

- **The two 200-fold RO brine samples of Cincinnati GAC contactor A; (code T4G2 and T4R6, Figure 2)**
- **All samples associated with Cincinnati GAC contactor D (Figure 3).**

Preparation for these samples consisted of volume reduction under nitrogen to 75 to 100 μl and addition of 1.8 μg of HEB internal standard.

Fractionation of Neutrals on Silica Gel. The samples fractionated on silica gel were the following:

- All samples associated with Cincinnati GAC contactor A except the two noted above
- The Super-Q reagent water blanks and pre- and post-lyophylization Cincinnati tap water samples
- The Jefferson Parrish XAD-2 concentrated samples.

The methylene chloride solution of neutrals remaining after removal of the acids was reduced in volume under nitrogen to about 100 μl in a 3.0 ml Chromaflex tube. About 500 μl of hexane was added and the volume reduced again to effect a solvent exchange. The neutrals were fractionated on a micro silica gel column (5% deactivated, about 0.5 cm by 7 cm) packed into a 6-inch disposable Pasteur pipet. The sample was eluted from the column using the following elution solvent sequence:

(1) application of the sample in 1.0 ml hexane

(2) 1.5 ml hexane elution (aliphatic fraction)

(3) 4.0 ml methylene chloride elution (combined aromatic and medium polarity fractions)

(4) 4.0 ml methanol elution (high polarity fractions).

The hexane, methylene chloride, and methanol fractions were evaporated under nitrogen (as above) to about 100 μl. The hexane and methanol fractions were used only for the determination of residue weights. The methylene chloride fraction was fortified with 1.8 μg of HEB internal standard and analyzed by glass capillary GC-MS. A minor modification to the fractionation scheme shown in Figure 4 was required by the Jefferson Parrish XAD-2 concentrated samples since for some of them the diethyl ether solvent had been reduced in volume to only 10 to 15 ml. Rather than reduce the sample volume further, risking loss of some moderately volatile materials, the sample was diluted to a standard, 15 ml volume with diethyl ether and partitioning of the acids was performed using a 25 ml separatory funnel. The remainder of the analytical scheme was the same as that shown in Figure 4 with the neutral fractionation on silica gel.

Process Blank for Sample Partitioning

A parallel and simultaneous process blank was generated and analyzed each time samples were partitioned. The blank sample consisted of 4.5 ml of re-distilled methylene chloride fortified with the deuterated internal standards (5.4 μg each corresponding to the 90 percent of the sample extracts which were partitioned).

GC-MS ANALYSIS

Gas Chromatography

The attempt to achieve extremely low detection limits required the use of high resolution gas chromatography. Wall-coated open-tubular glass capillary columns were prepared at Battelle for this purpose. Originally, in work with the extremely complex large-volume concentrates, all analyses were performed using two different liquid phases: SP1000 (polar) and SP2100 (nonpolar). These two types of coatings effectively complemented each other, so that compounds which co-eluted on one column were usually well separated on the other column. Also, some of the higher boiling compounds which did not elute from the polar column (SP1000) could be observed on the non-polar column (SP2100). The columns used in the first two years of the program were purchased from the J & W Scientific Company for which Supelco, Inc., Bellefonte, Pennsylvania, acted as distributor. The new analytical scheme for small-volume samples required only one GC phase, and the SP1000 phase was selected based on generally better performance for the compounds of interest and markedly superior ability to retain separating efficiency. The only significant compromise resulting from exclusive use of SP1000 columns was the inability to detect some high molecular weight compounds (for example, dioctyl phthalate and sebacate, abeitic and other resin acids and the two polynuclear aromatic hydrocarbon internal standards, (chrysene-D_{12} and perylene-D_{12}).

Before a capillary GC column was used for GC-MS analysis, the following minimum performance requirements were verified with GC-FID:

- For SP1000 columns (40 M, 0.25 mm I.D.) operated at 125°C with a helium carrier gas flow velocity of 20 cm/sec.

  (1) N_{eff} = 100,000 (C_{18}), minimum
  (2) SN = 25 (C_{17}-C_{18}), minimum
  (3) Decylaldehyde, no tailing
  (4) Decanol, no tailing
  (5) Acid/base ratio: 0.5 to 2.0
  (6) Sample capacity: 50 ng of C_{18}, no fronting

Figure 5 shows an example of a GC-FID chromatogram resulting from analysis of the standard GC test mixture of an acceptable SP1000 glass capillary column.

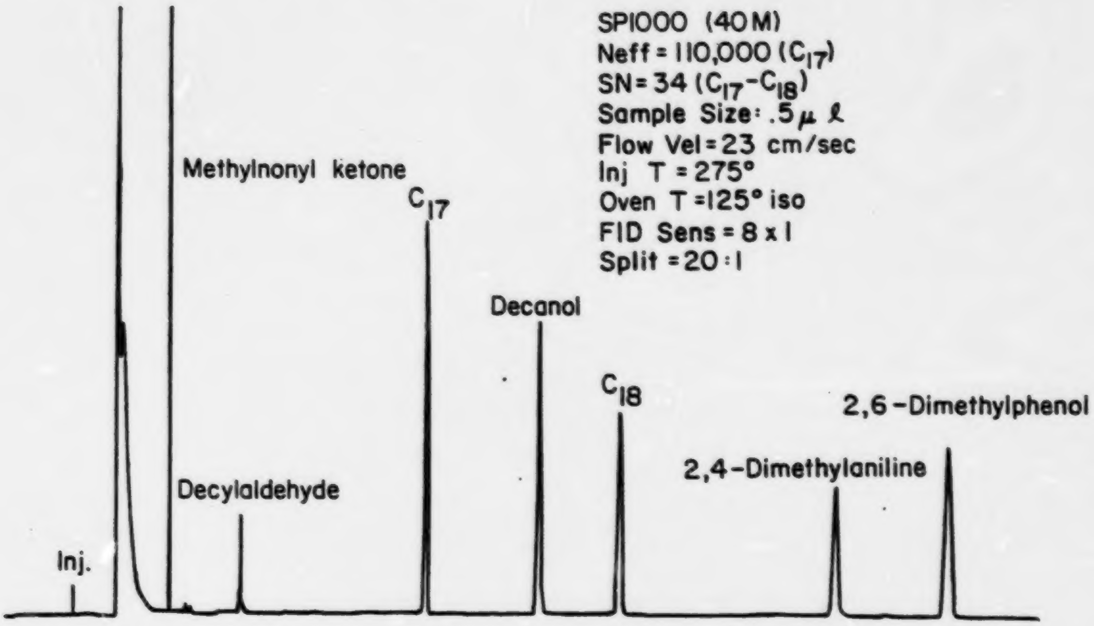

Figure 5. Typical performance validation chromatogram for a 40 meter SP1000 capillary column.

GC-MS Analysis Conditions

In order to achieve reproducible relative retention times and mass spectra over the three years of this project, certain GC and MS operating parameters were precisely reproduced for each GC-MS analysis. These standard GC-MS operating conditions are listed below:

Gas Chromatographic Operating Conditions for Finnigan 9500 GC

Injector temperature	250°C
Initial column temperature (hold)	50°C (6 min)
Temperature program rate	2°/min
Upper temperature limit	225°C
Injection volume	2 μl sample + 1 μl heptane
Transfer line temperature	250°C

Mass Spectrometer Operating Conditions for Finnigan 3200 With Systems Industries System/150 Data System.

Filament emission: 150 to 350 μA

Electron energy: 70 eV

Ion energy: 2 to 8 V (scan programmed)

Extractor voltage: 4 to 7 V

Lens voltage: -80 V

Signal amplification parameters:

Preamp setting: 10^{-8} amp/volt

Electron multiplier gain: 10^4

Scan acquisition parameters:

Mass range: 40-450 amu

Scan controlled by System/150 data system using the IFSS data acquisition program

IFSS parameters:

Maximum repeat count: 5

Samples/amu: 1

Repeat count before checking lower threshold: 2

Integration time: 2×10^{-3} sec

Lower threshold: 3

Upper threshold: 1

GC-MS analysis of the partitioned fractions and the unpartitioned concentrate, as well as their corresponding blank samples, provided the primary basis for identification and quantitation of organic compounds in the concentrate. To ensure high quality GC-MS data, the total GC-MS system performance was rigorously evaluated each day before beginning the sample analysis. GC-MS performance evaluation included the following operations:

(1) A check of the mass calibration by acquiring a spectrum of perfluorotributylamine (FC-43) using signal sampling at 0.1 amu intervals. This check was performed prior to every sample or blank analysis

(2) An evaluation of the mass spectrometer resolution and mass discrimination by analysis of decafluorotriphenylphosphine (DFTPP) according to the recommendations of Eichelberger, Harris, and Budde(5). This check was performed prior to every sample or blank analysis

(3) GC-MS analysis of a test mixture referred to as the Standard GC Separation Mixture (SGCSM). This mixture, analyzed once at the beginning of each day, was designed to evaluate the following performance characteristics:

- Proper MS sensitivity, resolution, and relative ion abundance
- Proper functioning of the splitless injection system
- Adequate capillary GC column efficiency
- Suitable capillary GC column neutrality (neither acidic nor basic)
- Absence of adsorptive sites or cold spots in the GC column and transfer line

COMPOUND IDENTIFICATION AND CONFIRMATION

Compounds were tentatively identified based on a computer or manual comparison of the compound mass spectrum with a library of reference mass spectra. Sample constituent mass spectra used for identification were corrected with an appropriate background spectrum subtraction, and they normally corresponded to the top of each discernible GC peak.

Three different mass spectral matching computer programs were available for use in the laboratory: two used a Systems Industries System 150 data system, and one used a Finnigan/Incos 2400 data system. Since the Finnigan/Incos mass spectral matching program correctly identified mass spectra more reliably than the other two programs and provided the most convenient data output format, all of the computer matching of mass spectra for small-volume samples was conducted on this system. The data base for the computer matching system included the most recently released mass spectral library from the National Bureau of Standards (31,357 spectra) plus additional spectra acquired at Battelle.

A compound identification was considered tentative unless it could be confirmed by comparison of the mass spectrum and relative retention time with the corresponding data obtained on an authentic reference sample analyzed under the same GC-MS conditions. The status of a compound's identification is indicated in the tabular computer output with either a "T" (for tentatively identified) or a "P" (for positively identified, i.e., confirmed). Compounds which were found in the blanks in approximately the same concentrations as in the samples were generally assumed to result from sample processing and are not reported as being present in the original concentrate. Every GC-MS sample data file was compared to the corresponding process blank data file on the basis of GC retention time and mass spectrum to ensure that no blank artifacts were reported as sample constituents.

ESTIMATATION OF SAMPLE CONSTITUENT CONCENTRATIONS

A semi-quantitative estimate of every identified compound was made using two methods involving comparison of the size of the GC peak of the compound the GC-MS reconstructed gas chromatogram (RGC) to that of the internal standard, HEB. The first method, which provided the relative size (RS) parameter, was developed for the highly complex large-volume samples and spanned a range of four orders of magnitude in GC peak size. The second method, expression of the GC peak size as a percentage of that for HEB, was more precise for the limited range of concentrations encountered for the small-volume samples. The Jefferson Parrish samples were the only ones for which the RS value GC peak size assignment were exclusively used.

The Relative Size (RS) Parameter

The relative size (RS) parameter is a somewhat imprecise but extremely cost-effective method for estimating the amount of each identified component. It is assigned on a logarithmic scale spanning four orders of magnitude, by visually estimating the size of each GC peak in the total ion current chromatogram relative to that of HEB, the internal standard added immediately before GC-MS analysis. In this work, each GC peak corresponding to an identified compound was assigned an RS value consisting of an integer from 1 to 9 on the basis shown in Table 2.

The computer report-generation software normalized all RS values to a typical large-volume (1514-liter) sample by the following equation

$$\text{RS (output)} = 2 \log_{10} \left[\frac{\text{antilog}_{10}[\text{RS(input)}/2]}{(\text{liters sampled})/(1514 \text{ liters})} \right] \qquad \text{Eq. 1}$$

RS value normalization, in theory, allows direct comparison from one concentrate report to another, regardless of the volume of water sampled. In practice, however, comparison between large-volume (greater than 1500 liters) and small-volume (10-liters) RS values is not recommended. The RS value is designed to provide approximate quantification for every water concentrate sample component identified. While it is tempting to assign the corresponding value in nanograms per liter of original water to each compound (as indicated in Table 2), such a correlation would be misleading and easily misinterpreted. The RS criteria will only provide exact quantification if the following conditions exist: (1) the sample component and internal standard have the same response factor for mass spectrometric detection, (2) instrument response is linear through the entire 10,000 fold RS range, (3) the sample component is recovered quantitatively through the partitioning scheme and suffers the same relative chromatographic losses as the internal standard, and (4) the component is removed from the original water into the extract quantitatively. Clearly the preceding conditions can never be met completely. However, since detection of the internal standard is expected to be reproducible, RS values for the same component can be directly compared from one sample to another with relative confidence.

Quantitative Approximation as Percentage of the Internal Standard, HEB

The research goals of the small-volume sample set include an evaluation of the performance of the RO concentration method and comparison of various high sensitivity methods of analysis. To meet these requirements, a more precise measurement of GC peak size than the half order of magnitude interval provided by the RS parameter was obviously required. This need was met by expressing the GC peak heights as a percentage of the peak height of the internal standard, HEB. These values, given as "% HEB" in the computer-generated tables, ranged from about 0.5 to 300 for the small-volume samples.

TABLE 2. GC PEAK RELATIVE SIZE (RS) VALUES FOR SEMI-QUANTITATIVE ESTIMATION OF COMPOUND CONCENTRATIONS

RS Value	GC Peak Size Relative to the Internal Standard[a]	Approximate Concentration[b]	
9	Greater than 100X	>1300 ng/l	1.3 ppb
8	30 to 100	.	.
7	10 to 30	.	.
6	3 to 10	.	.
5	1 to 3	13 ng/l	13 ppt
4	1/3 to 1	.	.
3	1/10 to 1/3	.	.
2	1/30 to 1/10	.	.
1	1/100 to 1/30	0.13 ng/l	0.13 ppt

a) The ranges are half orders of magniture so the RS value numbers span a "linear" log range. Technically, they should be 1-3.16, ...31.6-100, etc., but for visual comparison purposes only one significant figure is more appropriate.

b) Assuming the GC-MS response factor for the analyte to be equal to that of the Internal Standard and a 1514 liter (400 gallon) water sample. See text for other precautions concerning the use of the RS value.

c) ppb: parts per billion; ppt: parts per trillion.

QUALITY ASSURANCE

In the previous sections, a number of measures have been described which are designed to ensure that the data will consistently meet strict performance criteria. The following list summarizes those measures:

- Process blanks were generated concurrently for all sample extraction and fractionation procedures. These process blanks minimized the errors introduced by solvents, reagents, and sample handling
- Deuterated internal standards were used to monitor the sample extraction and partitioning process
- Anthracene was used to monitor activity of the silica gel used in the neutral separation chromatography
- Capillary columns had to meet a comprehensive list of minimum specifications before they were used for GC-MS data acquisition
- Decafluorotriphenylphosphine (DFTPP) was introduced to the mass spectrometer via a direct inlet to ensure proper ion source tune-up
- A standard GC separation mixture (SGCSM) was used to ensure that the complete capillary GC-MS computer system was functioning properly
- Compound identifications were confirmed by comparing the mass spectra and GC relative retention times to those obtained from authentic reference compounds
- All tenative identifications were inspected by an experienced mass spectrometrist to verify assignment

DATA MANAGEMENT

The great bulk of data generated by analyses of the large-volume concentrates and small-volume samples could not be managed efficiently by manual means. In addition, the needs for essentially unlimited flexibility in the correlation of compound identification results among any combination of samples required the development of a rather comprehensive computer data management system.

All of the data acquired by the dedicated GC-MS computer system (including the QC and blank analysis data) were transferred to magnetic tape for archival storage. Data relating to the characterization of identified compounds (i.e., the results of GC-MS data interpretation) were entered into a large, off-line computer located at the Battelle computer center. The following items were included for every identified compound.

- CAS number
- Common name
- Systematic name
- Industrial source and/or use
- Molecular weight
- Molecular formula
- Retention time
- Spectrum number
- Relative size of the GC peak, RS scale
- Relative size of the GC peak, % HEB scale
- Compound classification
- Functional group classification
- The fraction in which identification occurred
- The GC phase used

In addition to the above items relating to each identified compound, the following information was also entered into the master data base:

- Descriptive data on the sample
- Residue weight analysis data for the fractions
- Conditions used for the GC-MS analysis

The above items provided the necessary information for computer data processing and generation of the tables specified in Attachment "H" of the Scope of Work in the Request for Proposal for this project.

SECTION 6

RESULTS AND DISCUSSION

The analysis results of each of the four groups of samples enumerated in Section 4 are reviewed and discussed independently below. Some comparative discussion of the Cincinnati GAC contactor A and D sets of samples is also presented.

THIRTEEN SAMPLES ASSOCIATED WITH CINCINNATI GAC CONTACTOR A

Compound identification statistics for the thirteen samples associated with Cincinnati Waterworks GAC contactor "A" (January 14, 1980) are presented in Table 3. In all, 251 different compounds were identified in these thirteen samples although only 44 of these 251 were found in four or more of the samples. In addition, 9 of the 251 compounds are on EPA's "Consent Decree List" of priority pollutants and 13 are on the "Chemical Indicators of Industrial Pollution" list of the Federal Interim Primary Drinking Water Regulations (February 9, 1978). A key aspect of the work on large-volume concentrates was a reverse search of the GC-MS data for a set of 53 compounds designated by the Project Officer as having high potential health effect significance. Although cost restrictions did not allow reverse searching of the GC-MS data for these thirteen small-volume samples, 18 of the 54 compounds have nevertheless been identified. These compounds and their occurrences are as follows:

Compound	Code Names (see Table 3 and Figure 2) of Samples in Which Compound was Found
2,4,6-trichlorophenol	R4R5, T4R4
3,4-dichlorophenol	T4R5, T4R4, T4R3
1,4-dichlorobenzene	T4R4, T4E1, T4Y4
nitrobenzene	T4R3, T4Y4
2,4-dichlorophenoxyacetic acid	T4R1, T4E1, T4Y2, T4Y4
phenol	T4Y2, T4Y4
4-methylphenol	T4Y4
2-chloroaniline	T4R1, T4E1

A computer produced listings of all of the identified compounds for these thirteen samples is presented and discussed in a following section. This listing orders the compounds by decreasing size of the GC peak according to the

TABLE 3. COMPOUND IDENTIFICATION STATISTICS FOR THE THIRTEEN SAMPLES ASSOCIATED WITH CINCINNATI GAC CONTACTOR A

Sample Code	Description[a]	Number of Confirmed Identifications	Number of Identifications Remaining Tentative	Total Number of Identifications[b]	Number of Compounds Identified in Each Fraction		Number of Clearly Separated Compounds Unidentified[b]
					Acids	Neutrals	
T4R5	Pre-GAC, 100X Nyl, RO	19	17	36	36	0	9
T4R4	Pre-GAC, 10X Nyl, RO	25	18	43	27	16	10
T4R3	Pre-GAC, CA RO Permeate	39	51	90	48	42	12
T4R1	Pre-GAC, 10X CA, RO	12	18	30	17	13	14
T4R2	Pre-GAC, 100X CA, RO	14	20	34	28	6	13
T4R6	Pre-GAC, 200X CA, RO	21	25	46	16	30	24
T4E1	Pre-GAC	26	16	42	20	22	7
T4G1	Post-GAC	8	6	14	12	2	9
T4G2	Post-GAC, 200X RO	2	6	8	8	0	18
T4Y2	Pre-GAC XAD-2 Conc., ($SO_3^=$)	49	17	66[c]	36	30	12
T4Y4	Pre-GAC XAD-2 Conc.	57	21	78[d]	41	37	16
T4Y1	Pre-GAC XAD-2 Permeate ($SO_3^=$)	8	6	14	11	3	7
T4Y3	Pre-GAC XAD-2 Permeate	7	12	19	12	7	9

a) Abbreviations: GAC, granular activated carbon; RO, reverse osmosis; Nyl, Nylon RO membrane; CA, cellulose acetate RO membrane; 10X, 100X, 200X, the approximate factor for RO concentration; XAD-2 conc., the concentrated ether eluate of XAD-2 resin; ($SO_3^=$), the sample water was preserved by the addition of Na_2SO_3 before storage.

b) Compounds identified generically (i.e., alkanes, fatty acids, fatty alcohols, poly glycol ethers) but specifically enough to have known molecular weights are not entered into the computerized data base and, therefore, are not tabulated as confirmed on tentative identifications. In addition, these generic identifications are not counted as unidentified compounds since the confidence levels are always very high in these cases.

c) 16 of these compounds are known or suspected XAD-2 resin bleed artifacts.

d) 20 of these compounds are known or suspected XAD-2 resin bleed artifacts assigned RS values, and it is organized as a matrix showing the samples in which detections occurred by showing the %HEB value for each detection instance. In Appendix B, individual listings of the identified compounds are given for each of the thirteen samples.

Residue Weight Analysis

The results of residue weight analysis of the unpartitioned aliquots and the fractions are shown in Table 4. Only 10 percent of the organic extract was set aside for analysis as the unpartitioned concentrate, and the errors associated with residue weight determination of this small aliquot are considerably higher than those for the fractions. Thus, no primary conclusions are based on the unpartitioned aliquot data. It should be noted, however, that for the ten samples of Table 4 for which the comparison can be made, the unpartitioned aliquot indicates more organic material in the water than that indicated by the sum of the fractions. This result is consistent with the corresponding data for the large-volume concentrates presented in Volume 1. For example, in seven typical large-volume drinking water concentrates (composite extracts of RO brine), the average recovery of organic material into the fractions was only 52 percent.

Error limits have not been placed on the values in Table 4. Principally due to the very low amounts of material present, a rigorous treatment would result in relative error ranges in excess of 100 percent for a few values. The presentation of residue weight analysis results is not intended to carry a high degree of significance for the conclusions to be made in the discussions which follow. Indeed, determination of residue weights for samples is not required by the project Scope of Work and functions more as a quality control feature than a primary analytical result. The error component for the unpartitioned aliquot, due to the small size of the sample, was discussed above. Other aspects which enter into the overall error of residue weight analysis include:

- Although as much as 50% of the sample is consumed for residue weight analysis, the net residue can often be as low as 5 to 10 μg (especially for clean fractions and blanks). While the microbalance used for this work has a readout to the nearest microgram, its accuracy is probably at best ± 2 μg so that net weights carry an error of ± 4 μg. Thus, with aliquot factors ranging from 2 to 20, the uncertainty generated for calculated fraction weights after correction for the process blank can range from 16 to 160 μg from this source of error alone. For comparison, the neutral silica gel fraction net weights for these thirteen samples ranged from 4 to 180 μg.

- Original sample volumes are not measured, per se, but are read directly from the graduations of the Chromaflex tube in which they are stored. However, aliquots evaporated to produce the weighed residues are measured with syringes.

- Evaporated samples were not strongly heated before weighing so that medium volatility compounds would not be entirely lost. Since slow evaporation of these materials can begin before

TABLE 4. RESIDUE WEIGHT ANALYSIS RESULTS FOR UNPARTITIONED EXTRACTS AND FRACTIONS; CINCINNATI GAC CONTACTOR A

Sample Code	Description[a]	Volume of Water Represented by the Sample[b], liters	Amount of Material, as PPB in the Sample				
			Unpartitioned Aliquot[c]	Derivatized Acids	GC-MS Analyzed Neutral Fraction	Sum of Fractions Not Analyzed by GC-MS[d]	Sum of All The Fractions
T4R5	Pre-GAC, 100X Nyl, RO	16	--[e]	34	0.6	0.6	35
T4R4	Pre-GAC, 10X Nyl, RO	12	--[e]	52	0.3	77	130
T4R3	Pre-GAC, CA RO Permeate	10	--[e]	17	14	30	61
T4R1	Pre-GAC, 10X CA, RO	12	470	100	1.7	78	180
T4R2	Pre-GAC, 100X CA, RO	16	480	56	1	36	93
T4R6	Pre-GAC, 200X CA, RO	32	100	59	11[f]	--[f]	70
T4E1	Pre-GAC	10	320	17	5	107	130
T4G1	Post-GAC	10	310	3	5	14	22
T4G2	Post-GAC, 200X RO	32	31	2	2[f]	--[f]	4
T4Y2	Pre-GAC XAD-2 Conc., ($SO_3^=$)	10	380	89	18	49	160
T4Y4	Pre-GAC XAD-2 Conc.	10	340	99	14	56	170
T4Y1	Pre-GAC XAD-2 Permeate ($SO_3^=$)	10	350	3	1	1	5
T4Y3	Pre-GAC XAD-2 Permeate	10	110	40	3	6	49

a) Abbreviations: GAC, granular activated carbon; RO, reverse osmosis; Nyl, Nylon RO membrane; CA, cellulose acetate RO membrane; 10X, 100X, 200X, the approximate factor for RO concentration; XAD-2 conc., the concentrated ether eluate of XAD-2 resin; ($SO_3^=$), the sample water was preserved by the addition of Na_2SO_3 before storage.

b) Volumes indicated as 10 liters were precisely measured. The other volumes were calculated by multiplying the approximate RO factor by the measured volume of concentrate received for analysis. Thus, these calculated volumes carry the inaccuracy of the RO concentration factor.

c) Unpartitioned aliquots were only 10 percent of the sample and thus carry a greater relative error than the fractions.

d) Sum of the results for the aliphatic fraction (hexane silica gel eluate) and the highly polar fraction (methanol silica gel eluate).

e) Sample was accidently evaporated to dryness during concentration before GC-MS analysis.

f) Neutrals were not partitioned on silica gel (see Figure 4 for neutral fractionation option).

completion of solvent evaporation, a subjectivity element in instrument reading was thereby introduced.

- Methanol elution of silica gel always carried some stationary phase into the collected fraction, either from microcrystalline solid liberated by the strong methanol-silica gel interaction or from some minute solubility of silica gel in this solvent. As an example of the magnitude and variability of this background effect, residue weights of the methanol fractions of 28 typical process blanks averaged 340 μg with a standard deviation of 108 μg (32 percent).

- No correction was made for the amount of sample consumed in GC analyses prior to residue weight determinations.

Comparison of the residue weight values in Table 4 is addressed in the section below.

Comparison of Results Among the Thirteen Samples

Residue Weights--

The residue weight results for the sum of all the fractions, shown in Table 4, suggest a number of conclusions. The two samples of water taken after GAC contactor treatment, T4G1 and T4G2, show significantly lower levels (22 and 4 ppb, respectively) of organic material than the samples which represent water before GAC treatment. The 18 ppb difference between these two pre-GAC values is not considered significant. The two samples concentrated by XAD-2 resin, T4Y2 and T4Y4, are consistent with each other (160 and 170 ppb, respectively) and may indicate somewhat more efficient removal of organics by the resin than by direct liquid-liquid extraction (130 ppb for sample T4E1). They also indicate XAD-2 as the most effective extraction method for removal of acidic material with 89 and 99 ppb, respectively, recovered in these acid fractions. This effectiveness toward organic acid recovery would probably be reduced significantly without acidification to pH 2 before processing. The comparatively low recovery of acids by direct liquid-liquid extraction (17 ppb in T4E1) has no apparent explanation. Conversely, liquid-liquid extraction (107 ppb for T4E1) was apparently twice as effective as XAD-2 extraction (49 and 56 ppb for T4Y2 and T4Y4, respectively) in the recovery of the hexane and methanol elutions of silica gel. Since these fractions were not analyzed by GC-MS, the class of compounds responsible for this difference cannot be identified. However, experience with large-volume concentrates indicates that poly glycol ethers may account for the result. These compounds have high water solubility and probably low affinity for the extremely apolar, aromatic hydrocarbon surface of the XAD-2 resin. On the other hand, relatively effective extraction into the medium polarity, weak hydrogen-bonding solvent methylene chloride would not be surprising.

Comparing the total recovery values for the fractions of the XAD-2 extracts (T4Y2 and T4Y4) with their respective permeates (T4Y1 and T4Y3) indicates effective removal by XAD-2 resin of the organic material recoverable in the fractionation scheme. The derivatized acid fraction value for T4Y3 is probably higher than the true value since the compound identification statistics (Table 3) and GC-MS chromatograms indicate the acid fractions of T4Y1 and T4Y3 are not significantly different.

If the RO membranes were correctly functioning (i.e., retaining most of the organic material in the brine while contributing no artifactual organic material or irreversably adsorbing organic material) the pre-GAC residue weight values would be expected to assume the following order:

T4E1	$\geq$	T4R1 $\simeq$ T4R2 $\simeq$ T4R6	>	T4R3	$\geq$	T4R4 $\simeq$ T4R5
Feed Water		Cellulose Acetate Concentrates		Cellulose Acetate Permeate		Nylon Concentrates

In many cases, however, values under "Sum of All Fractions" for these samples in Table 4 are distinctly different from this expected order, and in some cases they are inconsistent with each other:

- The values for T4R1, T4R2 and T4R4 are expected to be approximately equal since they presumably represent the same sample of water at varying stages of RO concentration. Instead, they decrease with increasing concentration factor: 10-fold, 180 ppb; 100-fold, 93 ppb; and 200-fold, 70 ppb for T4R1, T4R2 and T4R6, respectively

- Similarly to the above argument, the values for T4R4 and T4R5 are expected to be equal. The main difference between these two samples is in the methanol silica gel fraction ("Sum of Fractions Not Analyzed by GC-MS"), with the value for T4R5 unexpectly low and the value for T4R4 unexpectly high. Since the residue weight results for the methanol silica gel fraction are the least reliable (as discussed above) no conclusions should be drawn here

- A surprisingly large amount of material was found in the cellulose acetate RO permeate, T4R3. This material either penetrated the cellulose acetate membrane or was contributed by it.

- Ideally, the sum of organic material recovered from the three points in RO processing (cellulose acetate concentrate, cellulose acetate permeate, and nylon concentrate) should be equal to that found in the original water (T4E1). The data of Table 4 are obviously not consistent with this prediction.

Inference, based only on the residue weight analyses above, regarding the performance efficiency of the RO system is not well founded. While the relative imprecision of the residue weight analysis cited above does not render the results useless in this regard, this source of error in combination with the approximate nature of the RO concentration factor (estimated by the Project Officer to be about 10%) does severely limit applicability. Some definite conclusions, however, can be made based on the discussion of the identified compounds which follows.

Identified Compounds--

The compound identification results for the GAC contactor A samples are presented in Table 5, in which 251 identified compounds are listed in decreasing order of the RS values of GC peaks. The display format of Table 5 is a matrix in which each identification instance is indicated by the GC peak size as a percentage of the internal standard, hexaethylbenzene (HEB). In similar tables for the large-volume concentrates, the display format corresponding to Table 5 showed identification status as either confirmed or tentative. Substitution of the "%HEB" parameter in Table 5 for the identification status indicator (P or T) thus requires the reader to consult the tables for each sample in Appendix B for compound identification status information.

With respect to two of the stated goals for this work (1. evaluation of the effectiveness of various stages of the RO process for concentrating organic compounds in water and 2. comparison of the effectiveness of RO concentration, XAD-2 resin adsorption/desorption and batch liquid-liquid extraction), the sampled DW contained less organic material than would have been desirable. This circumstance is illustrated by the fact that the large-volume, pre-GAC concentrate corresponding to this sampling (see Figure 2) obtained from solvent extraction of RO brine (concentrate T4C, see discussion in Volume 1) contained material equal to only 80 μg of organic material per liter of original water. This amount was less than all other large-volume drinking water concentrate except two: Poplarville, Mississippi, (essentially a process blank at 0.6 μg/l) and Seattle, Washington (37 μg/l). With this relatively low level of organic material in the sampled DW, one would expect there to be only a few species present at or above the 1 μg/l (1 ppb) level. The listings of Table 5 are completely consistent with this expectation. The internal standard, HEB, was added to fractions prior to GC-MS analysis in an amount corresponding to 0.2 ppb in the original water (100 percent recovery basis). Only 9 compounds of Table 5 have %HEB values of 100 or more, and these 9 compounds appear among the first 32 listings. In the first two pages (90 compounds) of Table 5, the magnitudes of the %HEB values were distributed as follows:

	Number of Entries with %HEB Values in the Indicated Range				
	≥ 100	99-50	49-20	19-10	9-0.5
page one	9	32	49	29	22
page two	0	1	8	31	60

Virtually all of the entries of Table 5 after No. 115 show %HEB values less than 10. Assuming 100 percent recovery and the same relative response for GC-MS detection as HEB, most of the identified compounds in the 13 samples are thus present in the 4 to 100 ppt range, in agreement with the above cited expectation. As the amount of a compound detected decreases, so also decreases the level of confidence with which conclusions based on occurrence can be made. Furthermore, compounds in the third and succeeding pages of Table 5 were generally found in only one to three samples. In most of these cases it is impossible to unambiguously ascribe the detection or nondetection of a compound

TABLE 5. COMPOUND IDENTIFICATION RESULTS FOR THE THIRTEEN SAMPLES ASSOCIATED WITH CINCINNATI GAC CONTACTOR A

EPA 18 CONCENTRATES PAGE 7

COMBINED CONCENTRATE REPORT (PART I.8)

CONC.(%HEB)

	COMMON NAME	T4R5	T4R4	T4R3	T4R1	T4R2	T4R6	T4E1	T4G1	T4G2	T4E1	T4Y2	T4Y4	T4Y1	T4Y3
1	1,3-DIMETHYL-2-(2-ISOPROPYLNYL)ETHYLC	54.0	48.0	45.0	84.0	15.0				17.0					
2	%BENZOIC ACID	45.0	25.0		70.0	32.0			16.0			200.0	130.0	120.0	20.0
3	10-OXO-UNDECANOIC ACID		34.0	480.0	134.0	44.0	5.0								
4	2-ETHYLHEXANOIC ACID	84.0	51.0			59.0						28.0	13.0	5.0	
5	%N-HEPTANOIC ACID	84.0	40.0	200.0	84.0	40.0			4.0				10.0		
6	2-ETHYL-3-METHYLMALEIC ACID	76.0		96.0	137.0	65.0	100.0	68.0	96.0	67.0	68.0	96.0	35.0	23.0	19.0
7	3,4-DIMETHYLBENZOIC ACID	60.0		197.0											
8	DEHYDROABIETIC ACID	81.0		74.0		100.0									
9	4-METHYLHEXANAL			250.0											
10	3,6-DIMETHYLOCTANOIC ACID (ISODECANOI			10.0	33.0		15.0			23.0					
11	CIS-1,3-DICHLOROCYCLOHEXANE			115.0											
12	3,4-DICHLOROBENZOIC ACID									107.0					
13	%METHYL BENZOATE											233.0	124.0	4.0	3.5
14	(2,5-DIMETHYLBENZENE)BUTANOIC ACID	28.0										7.0			
15	CLOFIBRIC ACID	3.0		5.0	22.0	12.0	29.0	11.0			11.0	9.0	8.0		
16	%AZELAIC ACID	15.0	7.0	70.0		15.0	13.0					30.0	50.0		
17	9-KETOCAPRIC ACID	47.0	11.0	75.0	35.0	20.0	12.0								
18	2-PYRROLIDONE	12.0	3.0	50.0											
19	2,3-DIMETHYLMALEIC ACID	22.0	9.0	35.0	57.0	44.0	10.0	40.0	88.0	98.0	40.0	22.0	18.0	20.0	18.0
20	5-HEXYLODIHYDROFURANONE	22.0		18.0		15.0									
21	%CAPROIC ACID		25.0			29.0							14.0		
22	10-UNDECENOIC ACID		11.0	19.0	14.0	19.0									40.0
23	2-ACETYL-P-TOLUIC ACID		22.0	38.0		27.0						5.0			
24	%+$0-DICHLORO BENZENE		2.0	9.0				5.0			5.0	60.0	52.0		
25	3-HEXANOL			53.0											
26	6-UNDECANOL			35.0											
27	1,2-OCTANEDIOL			40.0											
28	3-HYDROXYNONANOIC ACID			22.0	34.0	14.0	16.0								
29	2-NONENAL					16.0									
30	%BENZALDEHYDE						30.0					6.0	1.0		
31	1,3,5-TRIMETHYLCYANURIC ACID						116.0								
32	PALMITOLEIC ACID								80.0						
33	ETHYLENE GLYCOL, MONOMETHYL ETHER									35.0					
34	%PELARGONIC ACID											25.0	31.0		
35	%LAURIC ACID											74.0	83.0		
36	0-ETHYLBENZOIC ACID											10.0*	35.0*		
37	%MYRISTIC ACID											32.0	40.0		
38	%P-TOLUENESULFONAMIDE													2.0	35.0
39	%OLEIC ACID														92.0
40	HEXAN-3-ONE														45.0
41	%$M-XYLENE											22.0*	10.0*		
42	$ETHYLBENZENE											8.0	3.0		
43	ETHYL ISOPROPYL ETHER	11.0													
44	%PHTHALIC ACID	4.0				5.0						8.0*	8.0*		
45	4-(1,5-DIMETHYL-3-OXOHEXYL)LOHEXANECA	10.0	3.0						13.0						

(Continued)

TABLE 5. (Continued)

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COMBINED CONCENTRATE REPORT (PART I.B)

CONC.(%HEB)

	COMMON NAME	T4R5	T4R4	T4R3	T4R1	T4R2	T4R6	T4E1	T4G1	T4G2	T4E1	T4Y2	T4Y4	T4Y1	T4Y3
46	OCTAHYDRO-1,4A-DIMETHYL-1-PANTHRENE C	11.0	13.0	17.0		11.0	10.0			22.0					
47	4-METHYL-4-NITROPENTANOIC ACID	19.0		10.0											
48	ORTHO-TOLUIC ACID	5.0		10.0	80.0	6.0									
49%*+$2,4,6-TRICHLOROPHENOL		10.0	4.0												
50	O-CRESYL ACETATE	3.0	1.5	6.0		5.0	10.0	3.0			3.0		7.0		
51	%3,5-DICHLOROPHENOL	19.0													
52%*+$2,4-DICHLOROPHENOL		3.0	13.0	11.0											
53	ISOMYRISTIC ACID	5.0						4.0	4.0		4.0		11.0	1.0	4.0
54	ANISIC ACID	5.0		5.0				5.0			5.0	8.0			
55	%N-UNDECYLIC ACID		2.0	16.0											
56	2-ETHYL-3-METHYL-2-BUTENEDIOIC ACID		22.0												
57	ANTEISOHEPTADECANOIC ACID		11.0			7.0		6.0			6.0				
58	HEPTADECANOIC ACID		6.0		40.0			16.0			16.0				16.0
59	%CETYL ALCOHOL		12.0						20.0						
60	%BROMODICHLOROMETHANE		4.0	10.0				3.0			3.0				
61	%DIBROMOCHLOROMETHANE		6.0	27.0	1.0		7.0	27.0			27.0	14.0	10.0		0.5
62	%BROMOFORM		3.0	14.0	0.5			12.0			12.0	8.0	9.0		
63%*+$P-DICHLOROBENZENE			0.5					3.0			3.0		1.0		
64	O-NITROTOLUENE		2.0	15.0	0.5			8.0			8.0	7.0	1.0		
65	2,6-DINITROTOLUENE		2.0	10.0				5.0			5.0	3.0	5.0		
66	%1-METHYL-2,4-DINITROBENZENE		2.0	23.0	1.0			9.0			9.0	8.0	10.0		
67	4-HEPTANONE			18.0					9.0						
68	%BICHLORACETIC ACID			5.0				15.0			15.0	16.0	17.0		
69	%PHENYLACETIC ACID			6.0			6.0	4.0			4.0	13.0	16.0		
70	O-BROMOPHENOL			10.0											
71	TRIDECYLIC ACID			15.0				4.0	4.0		4.0				
72	SUBERIC ACID			16.0								6.0	8.0		
73	1,4-BENZOTHIAZIN-3-ONE			8.0											13.0
74	N-PHENYL ACETAMIDE			10.0										3.0	
75	OCTADECATRIENOIC ACID			9.0											
76	1,1-DICHLOROCYCLOHEXANE			10.0											
77	CIS-1-BROMO-2-CHLOROCYCLOHEXANE			24.0											
78	HEXACHLOROPENTANE			4.0	11.0	6.0		15.0	4.0		15.0			0.5	3.0
79%*+$NITROBENZENE				2.0									3.0		
80	%+NAPHTHALENE			9.6	22.0	6.0			2.5			11.0*	13.0*	3.0	3.5
81	4,8,12-TRIMETHYL-3,7,11-TRIATRIENITRI			18.0											
82	2-DODECENAL				26.0										
83	4-OXO-NONANOIC ACID				28.0				4.0						
84	ISOPENTADECANOIC ACID				20.0			14.0			14.0				7.0
85	%*2,4-DICHLOROPHENOXYACETIC AC, (2,4-D)				15.0			6.0			6.0	5.0	5.0		
86	DIVINYL MERCURY					2.0									
87	ISOPALMITIC ACID					4.0									
88	%DICAMBA					3.6	6.0								
89	3',4'-DIHYDROXYACETOPHENONE					9.0									
90	ANTEISOPENTADECANOIC ACID					9.0							3.0		

(Continued)

TABLE 5. (Continued)

COMBINED CONCENTRATE REPORT (PART I.0)

CONC.(XHEB)

	COMMON NAME	T4R5	T4R4	T4R3	T4R1	T4R2	T4R6	T4E1	T4G1	T4G2	T4E1	T4Y2	T4Y4	T4Y1	T4Y3
91	3-HYDROXYCAPRIC ACID					4.0									
92	DIMETHYL ISOPROPYL BENZENE						8.0								
93	2,5-HEXANEDIONE						9.0								
94	XTRIETHYL PHOSPHATE						7.0								
95	XN-METHYL-2-PYROLIDONE						8.0								
96	TRIPROPYLENE GLYCOL, METHYL ETHER						8.0								
97	TRIPROPYLENE GLYCOL, METHYL ETHER						7.0								
98	TRIPROPYLENE GLYCOL, METHYL ETHER						10.0								
99	TRIPROPYLENE GLYCOL, METHYL ETHER						7.0								
100	XBENZYL ALCOHOL						10.0								
101	5,6,7,7A-TETRAHYDRO-4,4,7A-METHYL-2(4						10.0								
102	TETRAPROPYLENE GLYCOL METHYL ETHER						16.0								
103	X7-OXABICYCLO(4.1.0)HEPTANE						29.0								
104	CYCLIC TETRAMETHYLENE ADIPATE						19.0								
105	2,2-DICHLOROETHANOL							24.0			24.0				
106	8,11-OCTADECADIENOIC ACID							28.0			28.0				16.0
107	2,2#-BI-1,3-DIOXOLANE							19.0			19.0	9.0			
108	DIETHYLENE GLYCOL									20.0					
109	XCAPRYLIC ACID											14.0	17.0		
110	XCAPRIC ACID											19.0	21.0		
111	P-ETHYLBENZOIC ACID											13.0*	12.0*		
112	PHENOXY ACETIC ACID											11.0	8.0		
113	ETHYLBENZALDEHYDE											13.0*			
114	X1,4-DIOXANE												39.0		
115	2-METHOXY-1-PROPANOL												13.0		
116	4-ETHOXYETHYLANILINE													10.0	
117	X1-BUTANOL	5.0													
118	3-METHOXY-3-METHYL-2-BUTANONE	4.0												2.0	
119	XMONOBUTYL PHTHALATE	5.0													
120	ANTEISOUNDECANOIC ACID	5.0													
121	M-TOLUIC ACID	6.0	3.0	8.0								3.0			
122	2-PHENYLPROPIONIC ACID	1.0	1.0									4.0			
123	XHYDROCINNAMIC ACID	7.0	3.0	4.0				4.0			4.0	7.0	5.0		
124	3,5-DIMETHYLBENZOIC ACID	4.0		7.0								7.0			
125	ANTEISOTRIDECANOIC ACID	3.0		9.0											
126	ISO-TRIDECANOIC ACID	5.0		5.0											
127	4-METHYL-2-PENTANOL		4.0												
128	P-TOLUIC ACID		2.0	5.0									3.0		
129	2-BUTYL THF		5.0												
130	XBENZYL CYANIDE		1.0	6.0	1.0			4.0			4.0				
131	TRIMETHYLNAPHTHALENE		1.5	4.0											
132	BROMOMETHANE			3.0											
133	2,4-DIMETHYLBENZOIC ACID			13.0											
134	O-ISOPROPYLBENZOIC ACID			5.0											
135	5-DODECANOL			8.0											

(Continued)

TABLE 5. (Continued)

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COMBINED CONCENTRATE REPORT (PART I.0)

CONC.(XHEB)

	COMMON NAME	T4R5	T4R4	T4R3	T4R1	T4R2	T4R6	T4E1	T4G1	T4G2	T4E1	T4Y2	T4Y4	T4Y1	T4Y3
136	2,5-DICHLOROPHENOL			2.0											
137	1,4-DICHLORO-2,5-DIHYDROXY BENZENE			4.0											
138	BENZONITRILE			5.0				3.0			3.0	2.0	3.0		
139	P			4.0									3.0		
140	3-CHLOROCYCLOHEXENE			5.0											
141	%ACETOPHENONE				1.0		3.5								
142	DIPROPYLENE GLYCOL METHYL ER (1-(2-						16.0								
143	%SALICYLIC ACID						11.0	3.0			3.0	6.0	3.0		
144	5-HEPTYL DIHYDRO-2-FURANONE						8.0								
145	P-ISOPROPYL BENZOIC ACID						8.0								
146	PROPYLENE GLYCOL MONOBUTYL ETHER						5.0								
147	N,N-DIETHYL FORMAMIDE						6.0								
148	HEPTYL ALCOHOL						5.0								
149	%CAMPHOR						5.0								
150	3-METHYL-2-CYCLOPENTEN-1-ONE						3.0								
151	5,5-DIMETHYL-2-FURANONE						6.0								
152	%TRIBUTYL PHOSPHATE						3.0								
153	DI-T-BUTYL ETHER						9.0								
154	4-HYDROXY-4-METHYLCYCLOHEXANONE						9.0								
155	2,2,6-TRIMETHYL-1,4-CYCLOHEXANEDIONE						7.0								
156	2-PHENYLBUTYRIC ACID							2.0			2.0				
157	%PROPIOPHENONE							5.0			5.0				
158	%PROPYL ALCOHOL											7.0			
159	%VALERIC ACID											7.0			
160	1-CHLORO-2-PROPANOL											9.0			
161	2,3,3-TRICHLORO-2-PROPENOIC ACID											6.0	5.0		
162	FUMAROYL CHLORIDE											6.0			
163	%*+PHENOL											6.0	1.5		
164	4-(1,5-DIMETHYL-3-OXOHEXYL)CYCLOHEXEN											8.0	11.0		
165	N-HYDROXYPHTHALAMIDE											6.0			
166	%$P-XYLENE											8.0*	2.0*		
167	%$O-XYLENE											10.0*	4.0*		
168	PSEUDOCUMENE											9.0*	4.0*		
169	METHYL P-ETHYLBENZOATE											5.0*	1.0*		
170	%*P-CRESOL												5.0		
171	1,4-DIHYDROXYTETRAMETHYLBENZENE												5.0		
172	4-ETHYLTETRAMETHYLPHENOL												5.0		
173	O-ANISIC ACID												10.0		
174	PENTADECANOIC ACID												4.0		
175	UNDECANEDIOIC ACID												7.0		
176	METHYL P-ETHYLBENZOATE												1.0*		
177	ADIPIC ACID, DIHEXYL ESTER												7.0		
178	DIOCTYLETHER												4.0		
179	DIETHYLENE GLYCOL, MONOMETHYL ETHER													3.0	
180	3-HYDROXY-1,2-BENZISOTHIAZOLE													5.0	7.0

(Continued)

TABLE 5. (Continued)

COMBINED CONCENTRATE REPORT (PART I.B)

CONC.(%HEB)

	COMMON NAME	T4R5	T4R4	T4R3	T4R1	T4R2	T4R6	T4E1	T4G1	T4G2	T4E1	T4Y2	T4Y4	T4Y1	T4Y3
181	%*O-CHLOROANILINE				1.0			3.0			3.0				
182	4-METHYLENE-1-(1-METHYLETHYYCLOHEXENE		2.0												
183	1-HEXANOL		1.0												
184	1,3-DIMETHYNAPHTHALENE		2.0												
185	1-ALLYLNAPHTHALENE		2.0												
186	TRIMETHYLNAPHTHALENE		0.5												
187	%$CUMENE			1.0											
188	%+$M-DICHLOROBENZENE			1.5				1.0			1.0				
189	%+$DICHLOROETHYL ETHER			1.0				1.0			1.0				
190	5-(PENTYLOXY)-2-PENTENE			1.5											
191	%HEXYL METHYL KETONE			1.0											
192	4-METHYLBENZALDEHYDE OXIME			1.0											
193	BUTYLBENZOATE			1.0											
194	P-NITROTOLUENE			3.0				1.5			1.5		1.0		
195	%2-ETHYL NAPHTHALENE			1.0											
196	1,6-DIMETHYLNAPHTHALENE			3.0											
197	%PHENYL ETHER			1.0				0.5			0.5				
198	ISOPROPYLNAPHTHALENE			1.0											
199	3-METHYLBIPHENYL			3.0											
200	4-METHYL BIPHENYL			2.0											
201	TRIMETHYLNAPHTHALENE			0.5											
202	3,3-DIMETHYLBIPHENYL			1.0											
203	4,4-DIMETHYLBIPHENYL			1.0											
204	[1,1#-BICYCLOPENTYL]-2-ONE			2.5											
205	1-ISOCYANONAPHTHALENE			2.0											
206	1-BROMO-2,3-DIMETHYLNAPHTHALENE			3.0											
207	1-METHYLFLUORENE			1.0											
208	3,5-T-BUTYL-4-HYDROXY-2,4-COHEXADIEN-			1.0											
209	1,1#-(3,3-DIMETHYL-1-BUTENYENE)BISBEN				0.5										
210	DIMETHYL ISOPROPYL BENZENE						1.5								
211	1,1,2-TRICHLORO-1-PROPENE						2.0								
212	2,6-BIS(1,1-DIMETHYLETHYL)-THYLPHENOL						3.0								
213	LEVULINIC ACID							6.0			6.0				
214	%LAURYL ALCOHOL								2.0						
215	1-ETHYL-3-METHYL BENZENE											3.0*			
216	%MESITYLENE											2.0*	0.5*		
217	ETHYL DICHLOROACETATE											1.0	1.0		
218	%ETHYL BENZOATE											3.0*	1.0*		
219	METHYL PALMITATE											1.0	2.0		
220	ETHYL PALMITATE											2.0	2.0		
221	1-METHYL-4-PROPYLBENZENE											2.0*			
222	1-ETHYL-3,5-DIMETHYL BENZENE											3.0*	11.0*		
223	1,2,3-TRIMETHYL BENZENE											3.0*	2.0*		
224	1-METHYL-2-PROPYL BENZENE											1.0*			
225	DIMETHYL ETHYL BENZENE											2.0*			

(Continued)

TABLE 5. (Continued)

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COMBINED CONCENTRATE REPORT (PART I.B)

CONC.(%HEB)

	COMMON NAME	T4R5	T4R4	T4R3	T4R1	T4R2	T4R6	T4E1	T4G1	T4G2	T4E1	T4Y2	T4Y4	T4Y1	T4Y3
226	DIMETHYL ETHYL BENZENE											2.0*			
227	4-ETHYL-1,2-DIMETHYL BENZENE											4.0*	2.0*		
228	%CHLOROACETIC ACID												3.0		
229	%META-CRESOL												2.0		
230	4-METHYLPHTHALIC ACID												2.0		
231	2-ETHYL-1,4-DIMETHYL BENZENE												1.0*		
232	1-ETHYL-2,4-DIMETHYL BENZENE												0.5*		
233	4-ETHYLSTYRENE												1.5*		
234	%2-METHYLNAPHTHALENE												1.0*		
235	METHYL STEARATE												1.0		
236	2,3,6-TRIMETHYLNAPHTHALENE			1.0											
237	4-PHENYLBICYCLOHEXYL				0.5										
238	%9H-FLUOREN-9-ONE				0.5										
239	1,2-DICHLOROCYCLOHEXANE				1.0										
240	3-HEPTANOL					0.5									
241	(1-METHYLUNDECYL)BENZENE					1.0									
242	%*ANTHRACENE					1.0									
243	1,4-DICHLORO-2-BUTENE					0.5									
244	(DICHLOROMETHYL)NAPHTHALENE							1.0			1.0				
245	%CYCLOHEXYL BROMIDE							1.0			1.0				
246	1,1,2,3-TETRACHLOROPROPANE							1.0			1.0				
247	2,4-DICHLORO-1-NITROBENZENE							0.5			0.5				
248	1,1,3-TRIMETHYL-3-PHENYL INDAN							0.5			0.5				
249	%3,4-DICHLOROANILINE												1.0		
250	%$TOLUENE														0.5
251	%9-METHYL ANTHRACENE														1.0

* DESIGNATES A POSSIBLE OR PROBABLE XAD-2 RESIN BLEED ARTIFACT

to variations in recovery and detection efficiencies, isolated introductions of artifacts, or genuinely unique occurrences. For this reason, most of the following discussion is based on the first 115 entries of Table 5 which are taken as the most significant for comparative purposes.

High-polarity compounds found in the neutral fraction of the 200-fold RO pre- and post-GAC samples--The neutral compounds of the 200-fold RO samples of pre- and post-GAC water (code names T4R6 and T4G2, respectively) were not fractionated on silica gel as were the other eleven neutral fractions of this set of of samples (see Figures 2 and 4). Thus, the GC-MS analyzed neutral fraction of these two samples contained material which would have been recovered in the methanol silica gel eluate, a fraction not analyzed by GC-MS for the other eleven samples. Twenty-six of the 30 neutral compounds identified in sample T4R6 (pre-GAC 200-fold RO) were not identified in the methylene chloride silica gel eluate of the other eleven samples. Since all 26 of these compounds contained the types of functional groups usually found in the high-polarity fraction, it is not surprising that they were not found in the samples for which this fraction was not analyzed. Similarly, the 200-fold RO post-GAC sample, T4G2, contained two compounds which could not have been observed in the 11 samples with silica gel neutral compound fractionation. The entries for these 28 compounds have been enclosed in parentheses in Table 5 to distinguish them from the neutral compounds of chemical types which could be recovered in the GC-MS analyzed neutral fractions of the other samples. The types of functional groups represented by the 26 and 2 compounds of T4R6 and T4G2, respectively, are poly glycol ethers, alcohols, ketones, lactones, amides, organic phosphate esters, polar ethers, aldehydes and polar nitrogen containing compounds.

Recovery effectiveness comparison of RO, XAD-2 resin and liquid-liquid extraction methods--A compound which was recovered about equally well by all three methods would be expected to be absent from the XAD permeates (T4Y1 and T4Y3) and the cellulose acetate (CA) RO permeate (T4R3) as well as the two nylon (NYL) membrane RO concentrates (T4R4 and T5R5), while reasonable (and comparable) recoveries would be observable for the XAD-2 concentrates (T4Y2 and T4Y4), the liquid-liquid extract (T4E1) and all three CA RO concentrates (T4R4, T4R5, and T4R6). In addition, lack of detection or detection at greatly reduced levels of the compound in both post-GAC samples would also be consistent with efficient operation of that treatment module. Of the first 115 compounds listed in Table 5 only clofibric acid (entry 15) shows the above ideal distribution among the 13 samples. XAD-2 recovery of this species was about the same as that for liquid-liquid extraction, and, of the small amount escaping the CA RO unit, a comparable amount was recovered in one of the two NYL RO samples. In addition, this commonly seen DW contaminant was not detected in either post-GAC samples (T4G1 and T4G2).

Two other compounds which are nearly always detected at relatively high levels in DW and AWT samples are dimethylmaleic acid and methylethylmaleic acid (entries 6 and 19, respectively). Although both of these compounds were detected in all 13 samples there is no possibility that they are artifacts introduced by sample extraction or fractionation procedures since they have never been detected in any process blank for either large-volume concentrates or small-volume samples. In contrast to most of the compounds of Table 5, GAC was essentially ineffective (see entries under T4G1 and T4G2) for the removal of these two acids; this result is undoubtedly due to the combination of high polarity and nearly complete ionization at the neutral pH of GAC contactor treatment (for example, the pK_a maleic acid is 2.0). Similarly, even at pH 2.0, major portions of these two compounds were not retained by the XAD-2 resin since about equal amounts were found in the XAD-2 concentrates and permeates (T4Y2 and T4Y4, and T4Y1 and T4Y3, respectively). RO retention of these compounds was no better than that for XAD-2 resin, with the CA RO permeate (T4R3) containing about the same concentrations of these two acids as all three CA RO concentrates (T4R1, T4R2, and T4R6). NYL RO retention was not significantly better than that for CA with less material recovered in the two NYL RO concentrates (T4R4 and T4R5) than the NYL RO feed (i.e., the CA RO permeate, T4R3). Since dimethylmaleic and methylethylmaleic acids were identified in essentially every large-volume concentrate, an early hypothesis during that work was that they were contaminants introduced by RO processing. Their observance in the small-volume samples not concentrated by RO (T4E1, T4G1, T4Y1, T4Y2, T4Y3, and T4Y4) unambiguously indicates these two compounds to be ubiquitous constituents of DW from surface water sources.

Benzoic acid was the only other compound found in all of the samples. The distinctly higher levels in the XAD-2 samples (T4Y2, T4Y4, and T4Y1) undoubtedly have some contribution from the resin since benzoic acid has been previously observed as an XAD-2 resin bleed artifact. In general, the GC peak size indications of Table 5 for benzoic acid are less precisely known than others since this compound usually eluted as a shoulder just prior to a variable but usually large peak for carbitol (used in the diazomethane generator and present as an artifact). In addition, the benzoic acid-D_5 internal standard slightly pre-eluted but did not separate from the native compound so that peak size correction for the deuterated component cannot be done precisely. However, the use of peak areas from extracted ion current profiles (EICP) of the deuterated and native compounds offers essentially perfect quantification of benzoic acid, and this has been done on a few selected data files. The amounts of native benzoic acid found were:

Sample	Description	Amount of Benzoic Acid
T4E1	pre-GAC DW	1.4 ppb
T4R2	CA RO 100-fold	0.9 ppb
T4R6	CA RO 200-fold	0.7 ppb
T4R3	CA RO Permeate	1.3 ppb
T4G1	post-GAC DW	0.2 ppb
T4G2	post-GAC; CA RO 200-gold	0.4 ppb
T4Y3	XAD-2 Permeate	4.5 ppb
Extraction blank, not methylated		0.05 ppb
Partitioning blank, methylated		0.02 ppb

These results indicate that GAC removed benzoic acid from water better than it did the more polar and stronger acids, dimethylmaleic and methylethylmaleic. The cellulose acetate RO membrane, however, appears to allow a sizable fraction of benzoic acid escape into the permeate. Quantification of phenol (entry 163, Table 5) has also been performed using the deuterated internal standard, phenol-D_5, for the same 9 analyses as above for benzoic acid. Phenol was detected by this method in all of the data files at levels ranging from 0.08 to 2.5 ppb. However, the levels found in three extraction blanks (0.8, 0.02, and 1.3 ppb) indicate that phenol is randomly present as an artifact at high enough levels to prevent data interpretation.

The haloforms, dibromochloromethane and bromoform (entries 61 and 62, Table 5, respectively) were identified in the pre-GAC water (T4E1) but not in either post-GAC sample (T4G1 and T4G2) indicating the GAC contactor was effective in removing these materials. Reasonable recoveries were also obtained for both XAD-2 concentrates (T4Y2 and T4Y1) with efficient absorption by the resin indicated by their absence in the two permeate samples, T4Y1 and T4Y3. The RO apparatus, however, did not retain these materials as well since a significantly higher concentration was observed in the cellulose acetate RO permeate (T4R3) than any of the RO concentrates, and neither compound was found uniformly in the RO concentrates. The relatively low concentrations of bromodichloromethane (entry 60) in samples T4E1, T4R3, and T4R5 may be present as a dichloromethane extraction solvent impurity. The most likely explanation for these observations is that the small molecular size of these haloforms allowed them to escape through the RO membrane. Other molecules which are significantly larger seem to display a similar behavior, however. For example, the nitroaromatics, o-nitrotoluene, 2,6-dinitrotoluene and 2,4-dinitrotoluene (entries 64, 65, and 66, respectively) and, at a lower confidence level, p-nitrotoluene (entry 194) were all detected in the pre-GAC sample, the XAD-2 concentrates and the RO permeate but were only poorly recovered, if at all, in the RO concentrates. All three isomers of dichlorobenzene (entries 24, 188, and 63) also display this type of behavior, although somewhat less definitively due to the very low concentrations found. The substantially higher levels found in the XAD-2 concentrates for 1,4-dichlorobenzene suggest that some amount of it may also be contributed by the resin as an artifact. Another compound which apparently was not retained by the RO membranes was dichloroacetic acid (entry 68). It was recovered essentially equivalently by the XAD-2 resin and pre-GAC liquid-liquid extraction, but found in the RO samples only in the cellulose acetate permeate.

Three chlorophenols, 2,4,6-trichlorophenol, 3,5-dichlorophenol, and 2,4-dichlorophenol, (entries 49, 51, and 52, respectively) may be artifacts contributed by the RO apparatus since they were identified only in the cellulose acetate permeate and nylon concentrates. A number of other compounds either found only or predominantly in the RO processed samples (and, thus, possibly contributed by the RO apparatus) or found in isolated instances at high levels are listed in Table 6 as possible artifacts from the RO apparatus or other unidentified sources.

TABLE 6. POSSIBLE ARTIFACT COMPOUNDS CONTRIBUTED BY THE RO APPARATUS AND OTHER SOURCES

Entry Number[a]	Compound Name	Samples Where Found[b]
APPARANT RO ARTIFACTS:		
1	1,3-dimethyl-2-(2-iso-propylphenyl)ethyl-cyclohexane carboxylic acid (a resin acid)	T4R5, T4R4, T4R3 T4R1, T4R2, T4G2
3	10-oxo-undecanoic acid	T4R4, T4R3, T4R1, T4R2, T4R6
5	n-heptanoic acid	T4R5, T4R4, T4R3, T4R1, T4R2, T4G1, T4Y4
8	dehydroabietic acid	T4R5, T4R3, T4R2
10	3,6-dimethyloctanoic acid	T4R3, T4R1, T4R6, T4G2
17	9-keto-capric acid	T4R5, T4R4, T4R3, T4R1, T4R2, T4R6
18	2-pyrrolidone	T4R5, T4R4, T4R3
20	5-hexyldihydorfuranone	T4R5, T4R3, T4R2
22	10-undecenoic acid	T4R4, T4R3, T4R1, T4R2, T4Y3
23	2-acetyl-p-toluic acid	T4R4, T4R3, T4R2, T4Y2
28	3-hydroxynonanoic acid	T4R3, T4R1, T4R2, T4R6
46	octahydro-1,4A-dimethyl-1-phenanthrene carboxylic acid (a resin acid)	T4R5, T4R7, T4R3, T4R2, T4R6, T4G2
48	o-toluic acid	T4R5, T4R3, T4R1, T4R2
APPARANT ARTIFACTS FROM UNKNOWN SOURCES:		
7	3,4-dimethylbenzoic acid	T4R5, T4R3
9	4-methylhexanol	T4R3
11	cis-1,3-dichlorocyclohexane	T4R3
12	3,4-dichlorobenzoic acid	T4G2
14	(2,5-dimethylbenzene)butanoc acid	T4R5, T4Y2
29	2-nonenal	T4R2
32	palmitoleic acid	T4G1
43	ethyl isopropyl ether	T4R5

a) The number corresponds to each compound entry number in Table 5.

b) See Figure 2 or Table 4 for correspondence of sample identities and and 4-digit code names.

SEVEN SAMPLES ASSOCIATED WITH CINCINNATI GAC CONTACTOR D

Special Interest Compounds and Compound Identification Statistics

Compound identification statistics for the 7 samples associated with the Cincinnati waterworks GAC contactor D are presented in Table 7. The sampling flow diagram identifying each of the 7 samples is shown in Figure 3. In all, 195 different compounds were identified in the 7 GAC contactor D samples; these compounds are listed in Table 9 which indicates the sample in which each compound was found by showing the size of each GC peak in %HEB units. Of the 195 compounds in Table 9, 51 compounds classified as XAD-2 resin bleed artifacts were found only in sample T5Y1 which is the only XAD-2 resin produced extract in this group of 7 samples. Thus, Table 9 contains a net total of only 144 compounds. Of these 144 compounds, 6 are members of the list of EPA semi-volatile Priority Pollutants and 7 are members of the "Chemical Indicators of Industrial Pollution" list of the Federal Interim Primary Drinking Water Regulations (February 9, 1978). Of the 53 compounds for which the large-volume concentrate data was searched (Table 4, Volume 1), 4 of those compounds have been detected by the standard data interpretation procedure (i.e., instead of by the computer search routine which was not used for these small-volume samples). Two of the search compounds, found in the pre-GAC sample T5E1, are probably significant detection instances: 2,4-D and nitrobenzene (entries 128 and 151, respectively, Table 9). The other two, p-cresol and 1,4-dichlorobenzene (entries 183 and 194, respectively) were found at very low levels in post-GAC samples and are probably not significant.

In Table 7, 54 of the 76 compounds identified in the only XAD-2 produced sample, T5Y1, are denoted definitely attributable as XAD-2 resin bleed artifacts. However, of the 22 compounds which cannot be unambignously attributed as artifacts, only 3 of them were identified in one of the other 6 samples. Thus, many of these 22 compounds may also be low level XAD-2 artifacts even though they are members of different chemical classes of compounds than those found to be frequently present as XAD-2 artifacts. Disregarding the entries in Table 7 for sample T5Y1, the compound identification statistics are clearly consistent with what one would expect for pre- and post-GAC water samples.

Residue Weight Analysis

The results of residue weight analysis of the unpartitioned aliquots and the fractions are shown in Table 8. Since only 10 percent of the sample was reserved for analysis as the unpartitioned extract, the errors associated with this small aliquot are considerably higher than those for the acid and neutral fractions. For a number of reasons, which are reviewed in the corresponding paragraphs of the preceding discussions covering the residue weight analysis of the Cincinnati GAC contactor A samples, the sources of imprecision in the residue weight determination of Table 8 are not well controlled. Thus, conclusions based on the results of Table 8 do not have as much significance as those based on the compound identification results.

The high values in Table 8 for the unpartitioned aliquot and the neutral fraction of sample T5Y1 are undoubted due to the high levels of XAD-2 resin bleed artifacts. The relatively low levels of material in these clean samples

TABLE 7. COMPOUND IDENTIFICATION STATISTICS FOR THE SEVEN SMALL-VOLUME SAMPLES ASSOCIATED WITH CINCINNATI GAC CONTACTOR D

Sample Code	Description[a]	Number of Confirmed Identifications	Number of Tentative Identifications	Total Number of Identifications[b]	Number of Compounds Identified in Each Fraction		Number of GC Peaks Unidentified[b]
					Acids	Neutrals	
T5R4	Pre-GAC, 200X CA, RO	22	11	33	17	16	14
T5E1	Pre-GAC	50	32	82	30	52	18
T5G1	Post-GAC	3	2	5	3	2	6
T5Y1	Post-GAC, XAD-2 Conc.	40	36	76[c]	28	48	6
T5R1	Post-GAC, 10X CA, RO	10	8	18	7	11	5
T5R3	Post-GAC, 200X CA, RO	4	8	12	0	12	3
T5R2	Post-GAC, 10X Nyl, RO	4	4	8	6	2	2

a) Abbreviations: GAC, granular activated carbon; RO, reverse osmosis; Nyl, Nylon RO membrane; CA, cellulose acetate RO membrane; 10X and 200X, the approximate factor for RO concentration; XAD-2 conc., the concentrated ether eluate of XAD-2 resin.

b) Compounds identified generically (i.e., alkanes, fatty acids, fatty alcohols, poly glycol ethers) but specifically enough to have known molecular weights are not entered into the computerized data base and, therefore, are not tabulated as confirmed on tentative identifications. In addition, these generic identifications are not counted as unidentified compounds since the confidence levels are always very high in these cases.

c) 54 of these compounds are known or suspected XAD-2 resin bleed artifacts.

TABLE 8. RESIDUE WEIGHT ANALYSIS RESULTS FOR UNPARTITIONED EXTRACTS AND FRACTIONS; CINCINNATI GAC CONTACTOR D

			Amount of Material, as PPB in the Sample			
Sample Code	Description[a]	Volume of Water Represented by the Sample[b], liters	Unpartitioned Aliquot[c]	Derivatized Acids	GC-MS Analyzed Neutral Fraction	Sum of the Fractions
T5R4	Pre-GAC, 200X CA, RO	32	101	(13)[d]	14	(29)[d]
T5E1	Pre-GAC	10	(nd)[e]	51	36	87
T5G1	Post-GAC	10	109	11	0.5	11.5
T5Y1	Post-GAC, XAD-2 Conc.	10	230	3	133	136
T5R1	Post-GAC, 10X CA, RO	12	(nd)[e]	17	3.5	20.5
T5R3	Post-GAC, 200X CA, RO	32	15	(0.0)[d]	0.6	(0.6)[d]
T5R2	Post-GAC, 10X Nyl, RO	12	(nd)[e]	(0.0)[f]	2.8	(2.8)[f]

a) Abbreviations: GAC, granular activated carbon; RO, reverse osmosis; Nyl, Nylon RO membrane; CA, cellulose acetate RO membrane; 10X and 200X, the approximate factor for RO concentration; and XAD-2 conc., the concentrated ether eluate of XAD-2 resin.

b) Volumes indicated as 10 liters were precisely measured. The other volumes were calculated by multiplying the approximate RO factor by the measured volume of RO brine received for analysis. Thus, these calculated volumes carry the inaccuracy of the RO concentration factor.

c) Unpartitioned aliquots were only 10 percent of the sample and thus carry a greater relative error than the fractions.

d) An anomalously high residue weight for the acid blank (655 μg) resulted in a low or negative (i.e., 0.0) value.

e) Unpartitioned aliquot was inadvertantly discarded before determination of residue weight.

f) The corresponding acid blank fraction residue weight exceeded the sample (83 μg for the blank and 64 μg for the sample.

resulted in sample residue weights for the acid fractions which are not enough greater than the usually encountered variability in the acid blank to allow meaningful comparison. However, this situation did not prevail for the neutral fractions, and the results shown in Table 8 (excluding that for sample T5Y1) are definitely consistent with the expectation of reasonably effective organic compound removal by the GAC contactor. A comparison of the neutral fraction results for two pre-GAC samples in Table 8, T5E1 and T5R4, indicates that the RO membrane may have failed to retain about half of the neutral materials present. This conclusion is supported by the compound identification results, below. A similar comparison of the neutral fraction residue weight results for the post-GAC samples, T5G1, T5R1, T5R3 and T5R2, may indicate that the RO apparatus (both the cellulose acetate and nylon RO units) initially contributed some neutral material to the water which was then lost on further processing just as for the pre-GAC sample T5R4. However, in this case the error limits of these residue weight results and the lack of appropriate replicates as well as data for the cellulose acetate permeate and 200-fold nylon brine make this conjecture highly tentative. Note, however, that the numbers of identified compounds in Table 7 for these neutral fractions presents a surprising parallel set of values.

Identified Compounds

As noted above, the compound identification results for sample T5Y1 which is the only XAD-2 produced sample of this set were so dominated by XAD-2 resin bleed artifacts that they cannot be used to compare the performance of XAD-2 organic compound extraction from water using RO or batch liquid-liquid extraction. However, there are some other comparisons that can be made between the sets of compound identification results shown in Table 9.

Comparison of samples T5R4 and T5E1 (pre-GAC 200-fold RO and pre-GAC 10-liter solvent extract, respectively) adds support to previous conclusions based on the Cincinnati GAC contactor A results (preceding discussion) and the results from the Cincinnati, 10/17/78, large-volume concentrates (Volume 1). This conclusion was that relatively small, apolar organic molecules either permeate the RO membranes with significant facility or they are absorbed by it. In comparing the results shown in Table 9, it is important to note that the %HEB values have not been corrected for the differences in volume which the various samples represent (these water volumes are shown in Table 8). Thus, in comparing the T5R4 and T5E1 results, %HEB values for the former must be divided by 3.2 or, alternatively, those for the latter multiplied by 3.2. There are 15 compounds in Table 9 which were found in both samples T5R4 and T5E1. Nine of those 15 compounds have %HEB values (after adjustment by the 3.2 factor) which are essentially equivalent within the limits of the method. Eight of those 9 compounds are relatively strong acids (Table 9 sequence numbers are given in parentheses): ethylmethylmaleic (17), dimethylmaleic (83), clofibric (25), m-toluic (103), p-toluic (104), hydrocinnamic (106), anisic (110) and phthalic (111). The compounds of which a substantial amount of material was lost during RO processing are all non-ionic: dibromochloromethane (18), trimethylcyanurate (20), bromoform (37) and tetrahydrotrimethylbenzofuranone (116). Since the RO processed sample, T5R4, represented 3.2 times as much water as the 10 liters extracted for sample T5E1, a noticably higher detection sensitivity would be expected for T5R4. Just the opposite was the case, with 67 of the compounds

TABLE 9. COMPOUND IDENTIFICATION RESULTS FOR THE SEVEN SAMPLES ASSOCIATED WITH CINCINNATI GAC CONTACTOR D

COMBINED CONCENTRATE REPORT (PART I.B)

ID MODE OR CONC.(%HEB)

	COMMON NAME	T5R4	T5E1	T5G1	T5Y1	T5R1	T5R3	T5R2
1	%BENZOIC ACID	20.0	102.0		63.0*			
2	4-ETHYLSTYRENE				3.0*			
3	1,3-DIETHYL BENZENE				994.0*			
4	3-ETHYLSTYRENE				*160.0*			
5	5-METHYL INDAN				*110.0*			
6	%BROMODICHLOROMETHANE		420.0					
7	1-ETHYL-3-METHYL BENZENE				480.0*			
8	1,4-DIETHYL BENZENE				970.0*			
9	1,2-DIETHYL BENZENE				475.0*			
10	DIETHYL TOLUENE				674.0*			
11	P-ETHYL-ISOPROPYLBENZENE				325.0*			
12	1-METHYL INDAN				465.0*			
13	2,4,6-TRIMETHYLSTYRENE				350.0*			
14	DIVINYLBENZENE				480.0*			
15	M-DIETHENYLBENZENE				360.0*			
16	%METHYL BENZOATE				575.0*			
17	2-ETHYL-3-METHYLMALEIC ACID	112.0	55.0					
18	%DIBROMOCHLOROMETHANE	14.0	229.0					
19	%ACETOPHENONE	119.0			65.0*		1.5	
20	1,3,5-TRIMETHYLCYANURIC ACID	156.0	196.0	1.0				
21	1,2-DICHLOROCYCLOHEXANE		168.0					
22	TETRALIN		49.0		225.0*			
23	%BCUMENE				*090.0*			
24	2-METHYLDECALIN				145.0*			
25	P-ETHYL TOLUENE				270.0*			
26	ETHYLDECALIN				128.0*			
27	O-ETHYLSTYRENE				275.0*			
28	2,4-DIMETHYL-1-SEC-BUTYLBENZENE				110.0*			
29	2-METHYL INDAN				140.0*			
30	4-METHYL INDAN				190.0*			
31	A PENTENYLBENZENE				180.0*			
32	1,1A,6,6A-TETRAHYDROCYCLOPROPA]INDENE				135.0*			
33	ADIPIC ACID, DIHEXYL ESTER				265.0			
34	ETHYL PALMITATE				7.0*			
35	2,3-DIMETHYLMALEIC ACID	83.0	24.0					
36	10-OXO-UNDECANOIC ACID	65.0						
37	%BROMOFORM	3.0	75.0				8.5	
38	%7-OXABICYCLO[4.1.0]HEPTANE	35.0						
39	2-ETHYL-4-METHYL-1,3-DIOXOLANE		25.0					
40	1-CHLORO-2,4-HEXADIENE		36.0					
41	DIISOBUTYL KETONE		44.0					
42	1-INDANONE		37.0					
43	%PHENYL ETHER		37.0					
44	%TRIBUTYL PHOSPHATE		38.0					
45	3-METHOXY-3-METHYL-2-BUTANONE			10.0	40.0			

(continued)

TABLE 9. (continued)

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COMBINED CONCENTRATE REPORT (PART I.B)

ID MODE OR CONC.(%HEB)

	COMMON NAME	T5R4	T5E1	T5G1	T5Y1	T5R1	T5R3	T5R2
46	X$M-XYLENE				68.0*			
47	SEC-BUTYL BENZENE				45.0*			
48	(1,1-DIMETHYLPROPYL)BENZENE				30.0*			
49	4-ETHYL-1,2-DIMETHYL BENZENE				25.0*			
50	1-ALLYLBENZENE				40.0*			
51	(1-ETHYL-2-PROPENYL)-BENZENE				40.0*			
52	XETHYL BENZOATE				85.0*			
53	ETHYLBENZALDEHYDE				90.0*			
54	METHYL P-ETHYLBENZOATE				40.0*			
55	2+-ETHYLACETOPHENONE				45.0*			
56	X2-METHYLNAPHTHALENE				60.0*			
57	X1-METHYLNAPHTHALENE				50.0*			
58	1,5-BIS(T-BUTYL)-3,3-DIMETHBICYCLO(3.				40.0*			
59	ETHYL STEARATE				35.0*			
60	ETHYL MYRISTATE				4.0*			
61	XPHENYLACETIC ACID	18.0	2.5					
62	3-HYDROXYNONANOIC ACID	30.0						
63	CLOFIBRIC ACID	25.0	10.0					
64	2,5-HEXANEDIONE	11.0						
65	DIPROPYLENE GLYCOL, METHYL ETHER	13.0						
66	TRIMETHYLNAPHTHALENE	11.0						
67	4-HYDROXY-4-METHYLCYCLOHEXANONE	10.0	3.0					
68	XCAPROIC ACID		20.0					24.0
69	XN-HEPTANOIC ACID		5.0					7.0
70	XMESITYL OXIDE (3-ISOHEXEN-2-ONE)		8.0					
71	XCHLOROBENZENE		9.0					
72	1,1-DICHLOROCYCLOHEXANE		26.0					
73	PERCHLOROETHANE		9.0					
74	X+$O-DICHLORO BENZENE		19.0				2.5	
75	CIS-1-BROMO-2-CHLOROCYCLOHEXANE		29.0					
76	+ISOPHORONE		18.0					
77	BENZONITRILE		16.0					
78	O-NITROTOLUENE		18.0					
79	XBENZYL CYANIDE		14.0					
80	3,4-DIHYDRO-1(2H)-NAPHTHALENONE		31.0					
81	$ETHYLBENZENE				29.0*			
82	X$P-XYLENE				24.0*			
83	4-METHYL-2-PENTANOL				15.0			
84	X$O-XYLENE				33.0*			
85	METHYL N-AMYL KETONE				23.0			
86	ETHYLENE GLYCOL, MONOMETHYL ETHER				18.0			
87	1,2-BUTANEDIOL				17.0			
88	O-ETHYLBENZOIC ACID				16.0*			
89	CYCLOPROPYLBENZENE				20.0*			
90	METHYLISOBUTYL BENZENE				16.0*			

(continued)

TABLE 9. (continued)

COMBINED CONCENTRATE REPORT (PART I.B)

ID MODE OR CONC.(XHEB)

	COMMON NAME	T5R4	T5E1	T5G1	T5Y1	T5R1	T5R3	T5R2
91	1,3,5-TRIETHYLBENZENE				25.0*			
92	2-ETHYL TETRALIN				25.0*			
93	N,N-DIETHYL-4-METHYL-2-PENTANAMINE				15.0			
94	1-PHENYL-3-BUTEN-2-ONE				15.0			
95	X4*-ETHYLACETOPHENONE				15.0*			
96	X2-ETHYL NAPHTHALENE				15.0*			
97	2-METHYL-1-HEXANONE					29.0		
98	3-METHOXYPENTANE					11.0		
99	5-HEXYLODIHYDROFURANONE					13.0		
100	CYCLIC TETRAMETHYLENE ADIPATE					10.0	9.0	
101	DIMETHYL ISOPROPYL BENZENE						10.0	
102	LEVULINIC ACID	7.0						
103	M-TOLUIC ACID	7.0	2.0					
104	P-TOLUIC ACID	5.0	1.5					
105	XSALICYLIC ACID	9.0						
106	XHYDROCINNAMIC ACID	9.0	3.5					
107	P-ETHYLBENZOIC ACID	5.0			7.0*			
108	3-HYDROXYOCTANOIC ACID	10.0						
109	O-ANISIC ACID	10.0			1.5			
110	ANISIC ACID	5.0	3.0					
111	XPHTHALIC ACID	5.0	1.5		7.0			
112	DIMETHYL ISOPROPYL BENZENE	5.0					1.5	
113	N,N-DIETHYL FORMAMIDE	9.0						
114	XCAMPHOR	6.0				3.0		
115	5,5-DIMETHYL-2-FURANONE	5.0						
116	5,6,7,7A-TETRAHYDRO-4,4,7A-METHYL-2(4	10.0	8.0					
117	1-METHYLFLUORENE	4.0						
118	DIPROPYLENE GLYCOL, METHYL ETHER	5.0						
119	XDICHLORACETIC ACID		3.0					
120	ORTHO-TOLUIC ACID		5.0			2.0		
121	2-PHENYLPROPIONIC ACID		2.0					
122	3-(P-TOLYL)PROPIONIC ACID		4.0					
123	2,4-DIMETHYLBENZOIC ACID		3.0					
124	2-ACETYL-P-TOLUIC ACID		3.5					
125	4-PHENYL PENTANOIC ACID		7.0					
126	X2-(4-CHLORO-2-METHYLPHENOXYOPANOIC AC		2.5					
127	4-(1,5-DIMETHYL-3-OXOHEXYL)LOHEXANECA		2.0					
128	X*2,4-DICHLOROPHENOXYACETIC AC, (2,4-D)		3.0					
129	4-CHLOROCYCLOHEXENE		3.0					
130	CYCLOHEPTANONE		7.0					
131	2-METHYL-2-CYCLOPENTEN-1-ONE		7.0					
132	DICHLOROACETONITRILE		2.0					
133	1,1,3-TRICHLORO-1-PROPENE		3.0					
134	X*M-DICHLOROBENZENE		3.0					
135	3-METHYL-2-CYCLOPENTEN-1-ONE		3.0					

(continued)

TABLE 9. (continued)

COMBINED CONCENTRATE REPORT (PART I.B)

ID MODE OR CONC.(%HEB)

	COMMON NAME	TSR4	TSE1	TSG1	TSY1	TSR1	TSR3	TSR2
136	%+$DICHLOROETHYL ETHER		5.0					
137	3-PROPYLCYCLOPENTENE		4.0					
138	FENCHYL ALCOHOL		5.0					
139	%TRIETHYL PHOSPHATE		6.0			3.0	2.0	
140	TRIPROPYLENE GLYCOL, METHYL ETHER		5.0					
141	TRIPROPYLENE GLYCOL, METHYL ETHER		9.0					
142	TRIPROPYLENE GLYCOL, METHYL ETHER		7.0					
143	TRIPROPYLENE GLYCOL, METHYL ETHER		6.0					
144	DIPROPYLENE GLYCOL, 2-PROPENYL ETHER		5.0					
145	HEXACHLOROPENTANE		7.0					
146	1,2,3,4-TETRAHYDRO-1-NAPHTHALENONE		5.0					
147	TETRAHYDRO-1,1-DIOXIDE THIOPHENE		5.0					
148	N-(4-CHLOROPHENYL)ACETAMIDE		9.0					
149	PHTHALIDE		4.0			1.0		
150	%1-METHYL-2,4-DINITROBENZENE		7.0					
151	%*+$NITROBENZENE		30.0					
152	1,4-DICHLORO-2-BUTENE		2.0					
153	BENZILIDENEACETONE		6.0					
154	DIBUTYL SULFITE			5.0				
155	BENZOTHIAZOLE			6.0		12.0		
156	%CAPRIC ACID				6.0			
157	ETHYL LAURATE				6.0*			
158	4-HYDROXYACETOPHENONE				4.0			
159	%AZELAIC ACID				7.0			
160	%MONOBUTYL PHTHALATE				9.0			
161	2-ETHYLHEXANOIC ACID					7.0		10.0
162	%ETHYL ACETATE					5.0		
163	1,3-DIMETHYL-2-(2-ISOPROPYLNYL)ETHYLC					8.0		7.0
164	P-(1,1,3,3-TETRAMETHYLBUTYL)PHENOL					4.0		
165	P-(1-METHYLOCTYL)PHENOL (ANYL PHENOL					4.0		
166	2-NONENAL					6.0		
167	%+NAPHTHALENE					8.0		7.0
168	CIS-1,3-DICHLOROCYCLOHEXANE						3.0	
169	%$DIMETHYL PHTHALATE						2.0	
170	2,6-BIS(1,1-DIMETHYLETHYL)-THYLPHENOL						5.0	
171	LEVOPIMARIC ACID							3.0
172	NONYLPHENOL							6.0
173	2,2-DIMETHYLVALERIC ACID	1.0						
174	2-METHYLCAPRYLIC ACID	1.5						
175	DIVINYL MERCURY	1.0						
176	3,6-DIMETHYLOCTANOIC ACID (ISODECANOI	2.0						
177	%P-CHLOROBENZOIC ACID	1.0						
178	3-PHENYL PENTANOIC ACID	2.0						
179	4-BUTOXYBUTYRIC ACID	2.0						
180	$O-CHLOROPHENOL	0.5						

(continued)

TABLE 9. (continued)

COMBINED CONCENTRATE REPORT (PART I.8)

ID MODE OR CONC.(XHE8)

	COMMON NAME	T5R4	T5E1	T5G1	T5Y1	T5R1	T5R3	T5R2
181	N-PHENYL ACETAMIDE		42.0					
182	%9H-FLUOREN-9-ONE		1.0					
183	%*P-CRESOL			2.0				
184	%CAPRYLIC ACID				3.0			
185	%META-CRESOL				2.0			
186	3,4-DIMETHYLPHENOL				1.0			
187	DIETHYLENE GLYCOL, MONOMETHYL ETHER				2.0			
188	DIPROPYLENE GLYCOL				1.0			
189	METHOXY TOLUIC ACID				1.5			
190	1,3-DIOXALANE METHANOL				3.0			
191	DIMETHYL ISOPROPYL BENZENE						1.5	
192	%STILBENE OXIDE						2.0	
193	ISOPIMARIC ACID							4.0
194	%*+$P-DICHLOROBENZENE					1.0		
195	%FURFURAL					1.0		

* DESIGNATES A POSSIBLE OR PROBABLE XAD-2 RESIN BLEED ARTIFACT

identified in T5E1 not found in T5R4 while only 18 of the compounds found in T5R4 were not found in T5E1. Most of the compounds found in T5E1 but not found in T5R4 were relatively apolar or moderately polar species while 9 of the 18 compounds found in T5G4 but not found in T5E1 were acids or highly polar species (i.e., dimethylformamide and 2,5-hexanedione). These results are in agreement with the enhanced recovery expected for ionic or highly polar species which are strongly solvated and are, therefore, more efficiently retained by the RO membrane due to the larger molecular size of the species with its tightly associated solvation sphere. Examples of the 67 compounds found in T5E1 but not in T5R4 include: bromodichloromethane (6), dichlorocyclohexane (21), tetralin (22), diisobutyl ketone (41), 1-indanone (42), diphenyl ether (43), chlorobenzene (71), 1,2-dichlorobenzene (74), benzonitrile (77), 2-nitrotoluene (78), benzylcyanide (79), dichloroacetonitrile (132), 1,3-dichlorobenzene (134) and bischloroethyl ether (136).

The effectiveness of GAC contactor D for removing organic material from the sampled DW is obvious from Table 9. Only one compound, trimethylisocyanurate (20), was found in both concentrates T5E1 and T5G1 (10-liter per-GAC and post-GAC extractions, respectively), and the %HEB values were 196 and 1, respectively. Only 5 compounds were found in sample T5G1, and the %HEB values for these were all comparitively low (10, 6, 5, 2 and 1). Six compounds were found in both the T5E1 sample and one of the three post-GAC RO samples (T5R1, T5R2 and T5R3), but none of them were found in more than one of the three RO samples. Indeed, there is little agreement among the three post-GAC RO samples, with only 4 of 22 compounds found in any two of these three samples. Of course, the post-GAC water was nearly free of organic contamination, and, thus, many of these compounds (all of which were found at low levels, 10 to 1 %HEB) were probably artifacts contributed by the RO apparatus. Among the 22 compounds identified were 3 resin acids, 4 alkylated phenols (C_8 or greater) and two plasticizers. Computer-printed tables for each of the 7 samples are presented in Appendix C.

COMPARISON OF CINCINNATI GAC CONTACTOR A AND GAC CONTACTOR D RESULTS

Only 2 of the 13 GAC contactor A samples were prepared from post-GAC DW. Thus, 11 of the 13 samples contained reasonably high levels of organic material. In contrast, only 2 of the 7 GAC contactor D samples were prepared from pre-GAC DW. Thus, only 2 of these samples contained appreciable numbers of detectable organic species. The disparity in numbers of identified compounds between these two sample sets is, therefore, not surprising: 226 identified compounds for the 13 GAC contactor A samples and 144 compounds for the 7 GAC contactor D samples.

The T4G2 (Table 5) and T5R3 (Table 9) samples both correspond to post-GAC water concentrated to the 200-fold brine stage by RO. Similarly, the T4G1 (Table 5) and T5G1 (Table 9) samples both correspond to 10-liter extractions of post-GAC contactor water. Comparison of the two sets of data for the 200-fold RO concentrated samples shows that the GAC contactor A sample, T4G2, contained slightly fewer compounds than the contactor D sample, T5R3, (8 versus 12) but that they were at higher levels (22 to 110 versus 1.5 to 10, %HEB). In addition, all 8 T4G2 compounds were identified in the acid fraction while all 12 of the T5R3 compounds were identified in the neutral fraction. Comparison of the two sets of data for the post-GAC 10-liter extraction samples again shows the contactor A sample, T4G1, to contain predominantly acids and higher levels of compounds (the average %HEB value for the 14 compounds is 25) while the GAC contactor D sample, T5G1, again contained no acids and lower levels of compounds (the average %HEB value for the 5 compounds is 5). These results indicate that GAC contactor D was more effective at removing organic material from the finished DW than was contactor A. This result is not surprising, since, at the times the samples were collected at each unit, contactor A had been in service for 7 weeks while contactor D had been in service only 2 weeks. It is noteworthy also that the results for samples T4G1 and T4G2 (contactor A) indicate that relatively strong acids (for example, the di-acids methylethylmaleic acid and dimethylmaleic acid) are among the compounds for which GAC adsorption capacity diminishes earlier than other, less water soluable materials.

ANALYSIS RESULTS FOR THE 10-LITER EXTRACTION PROCESS BLANK

The liquid-liquid extraction procedure described under "Experimental" was designed to provide the most artifact-free performance possible at the 0.1 ppb level. The main features of the procedure were:

- Distillation of extraction solvent
- Use of EPA/HERL-CI-produced "Super-Q" reagent water
- Sample extraction in the sampling vessel
- Exposure of the sample water and extraction solvent to only glass surfaces, except for the Teflon-coated stir-bar
- Overnight heating at 450°C immediately prior to use of all glassware followed by protection from the laboratory environment while still hot
- Heating twice at 450°C of anhydrous sodium sulfate used to dry extracts.

The procedure for producing the extraction blank is described in Section 5. One to four samples were extracted as a set with a simultaneous extraction blank. In all, thirteen such sets were processed for the 10-liter extraction samples. All of the GC-MS data from the extraction process blank of each set were reviewed at the computer terminal by the project team member responsible for compound identification confirmation. The GC-MS data of the earlier extraction process blanks were carried through the usual routine of mass spectrum plotting and computerized library matching. In later work, since the extraction process blanks were relatively clean and reproducible, inspection of the data at the computer terminal without library matching and mass spectrum plotting was sufficient to monitor the extraction performance. In each case, the analyst labeled the significant peaks on a plot of the GC-MS RGC. Two typical examples of these extraction process blanks are shown in Figures 6 and 7. The dibutylphthalate peak in Figure 7 is an example of the highest level of phthalate contamination encountered. In a few cases, fatty acid contamination--generally present at very low levels--resulted in peak heights about equal to those for the internal standard, hexaethylbenzene. No other contaminants at significant concentrations were routinely encountered.

Since the recovered deuterated internal standards were added to the reagent water at the 0.6 ppb level, it is clear from inspection of Figures 6 and 7 that most of the contaminants were present at the 0.1 ppb level or lower. Especially noteworthy are the relatively low levels in the early eluting portion of the chromatogram of the usually encountered solvent impurities with chloroform the only extraction solvent contaminant present at relatively high levels. This necessary performance characteristic could only be obtained by careful redistillation of the methylene chloride extraction solvent. In addition, the GC peak heights of the recovered deuterated internal standards were highly consistant and reproducible in their ratios with each other and with the pre-analysis internal standard, hexaethylbenzene. Thus, the recovery efficiencies for the deuterated internal standards (and, presumably for the organic sample constituents, also) were relatively uniform for all samples.

At the compound identification confirmation stage of GC-MS data interpretation, the responsible analyst (who was the same individual as the one who reviewed all the extraction process blank data at the computer terminal) identified the sample constituents which were probable or possible artifacts of the extraction procedure. These known artifacts were not entered in the computer data base.

VALIDATION OF THE 10-LITER LIQUID-LIQUID EXTRACTION PROCEDURE

Reagent Water Samples

As noted above, the HERL-CI laboratory provided reagent water that was extraordinarily free of organic compounds. The method used by HERL-CI to prepare this reagent water (denoted Super-Q water) is described in Section 5, Analytical Scheme, Reagent Water. Two 10-liter Super-Q reagent water samples, fortified only with the 13 deuterated internal standards, were extracted on different days (4-day interval) as the first phase of validation of the 10-liter extraction method. The extracts were processed through the fractionation scheme (Figure 4) using the option for silica gel fractionation of the neutrals. The usual fractions (acid and neutral fractions and 10 percent unpartitioned aliquot) were analyzed by GC-MS as described in the analytical scheme. The GC-MS data were processed exactly as for the samples except that the compound identification results were not entered in the computer data base. The compound identification,results, in the form of labeled GC-MS chromatograms for these two samples, coded S1Q and S2Q, are presented in Appendix C. For each sample, the peaks in the GC-MS chromatograms are labeled to correspond to the entries in an accompanying table. This mode of presentation conveys more information than computer-printed tabulations such as Tables 5 and 9 since the

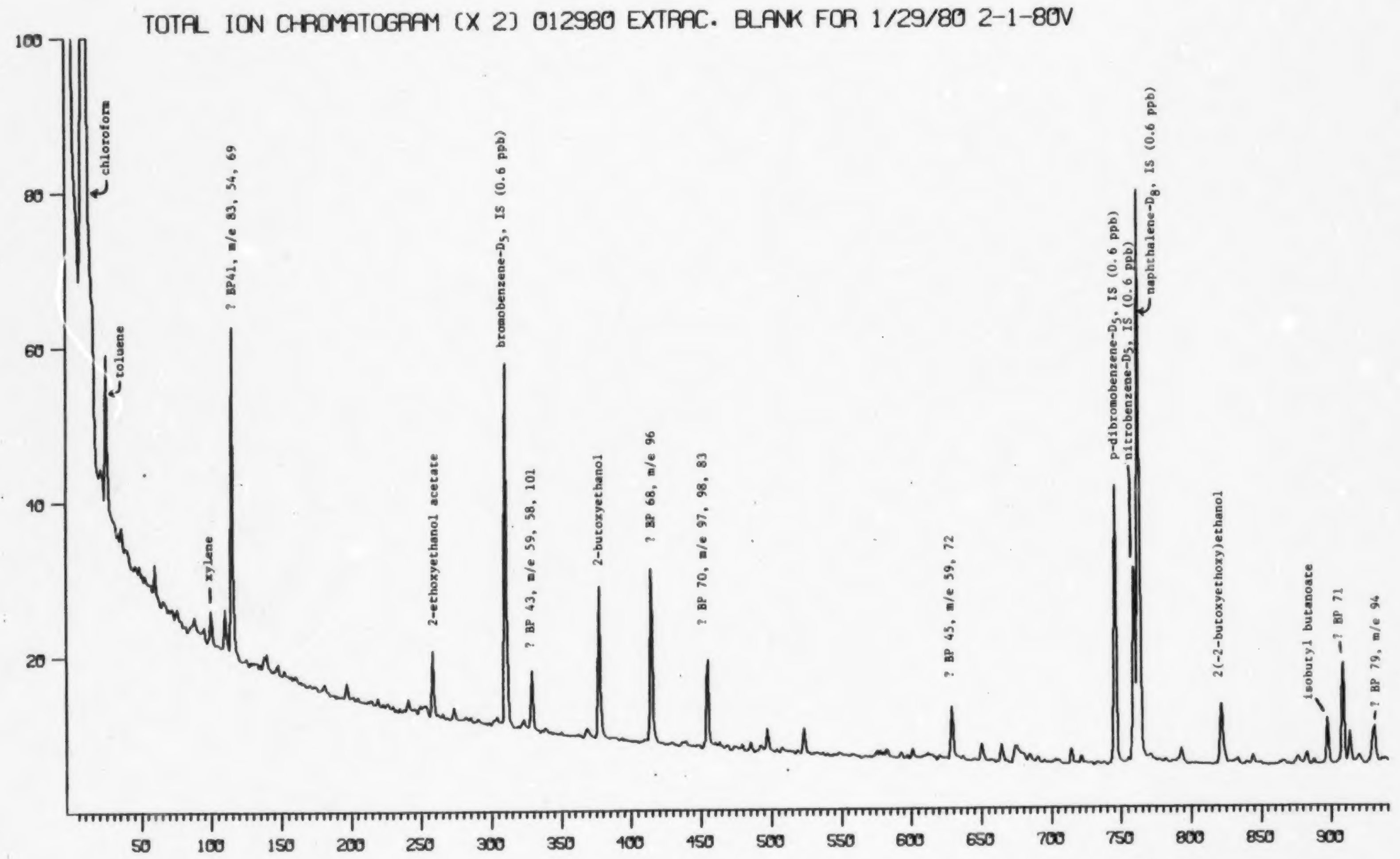

Figure 6. GC-MS chromatogram of a typical extraction blank showing relatively low levels of phthalate contamination.

(continued)

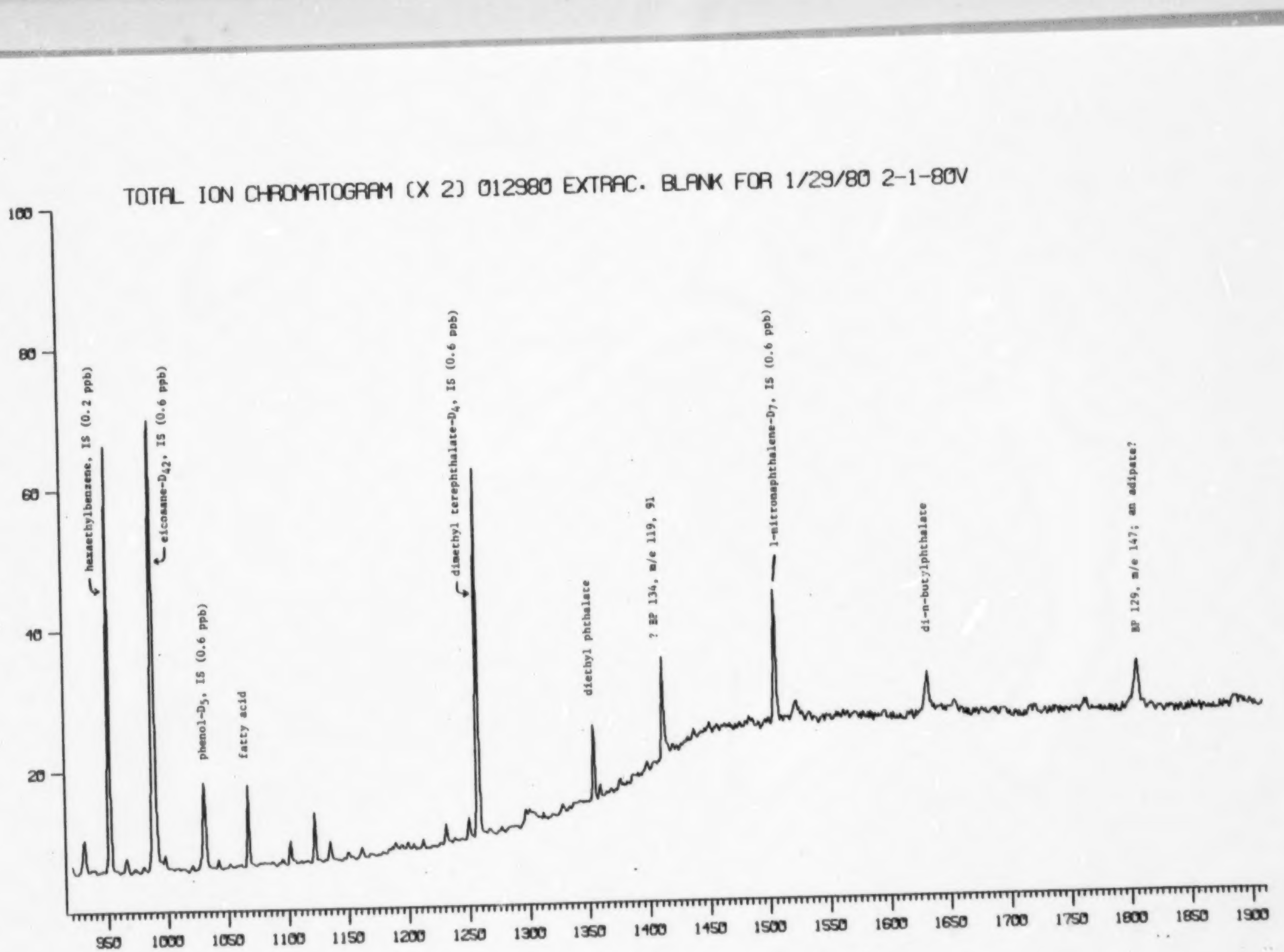

Figure 6. (continued)

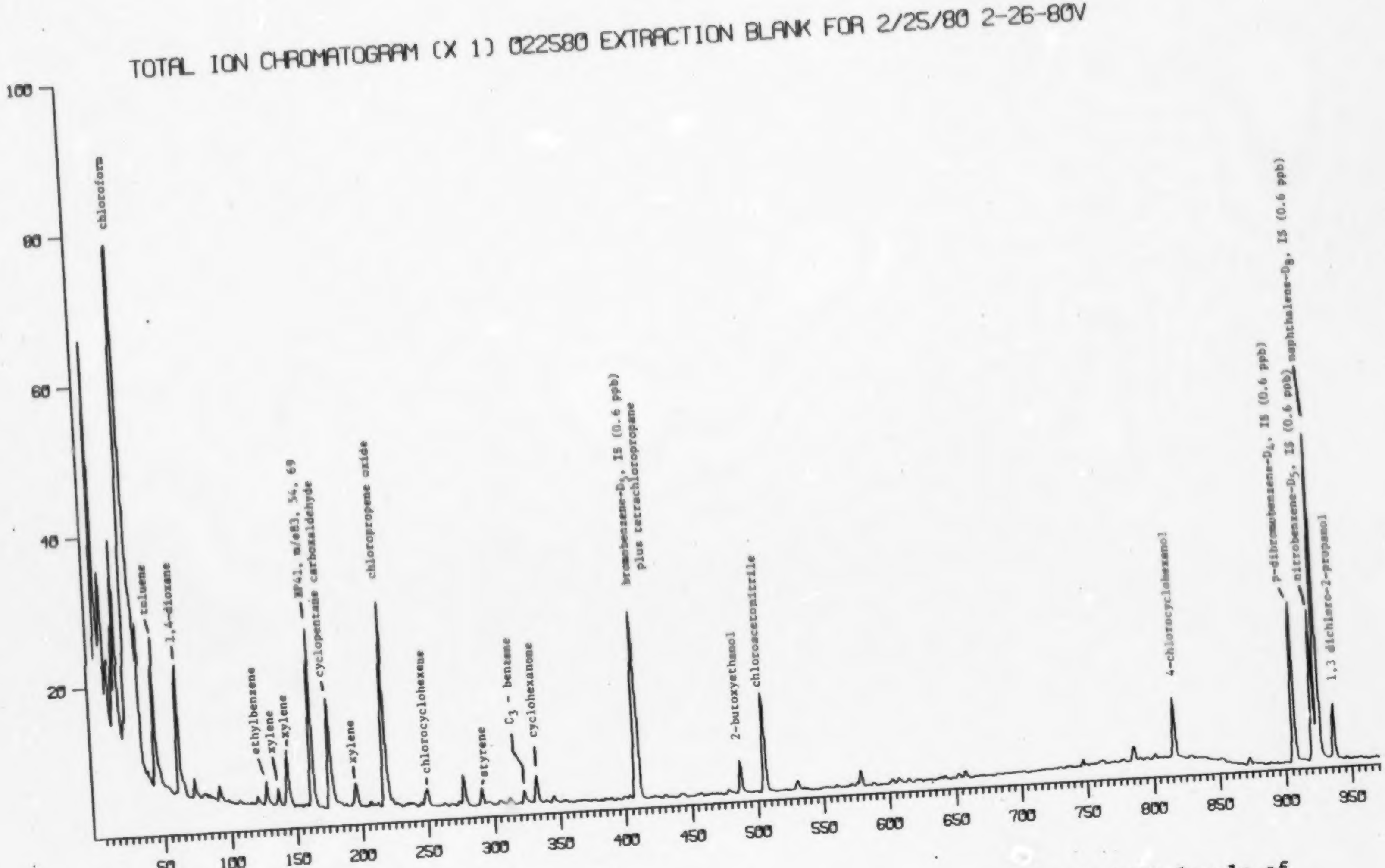

Figure 7. GC-MS chromatogram of a typical extraction blank showing relatively high levels of phthalate contamination.

(continued)

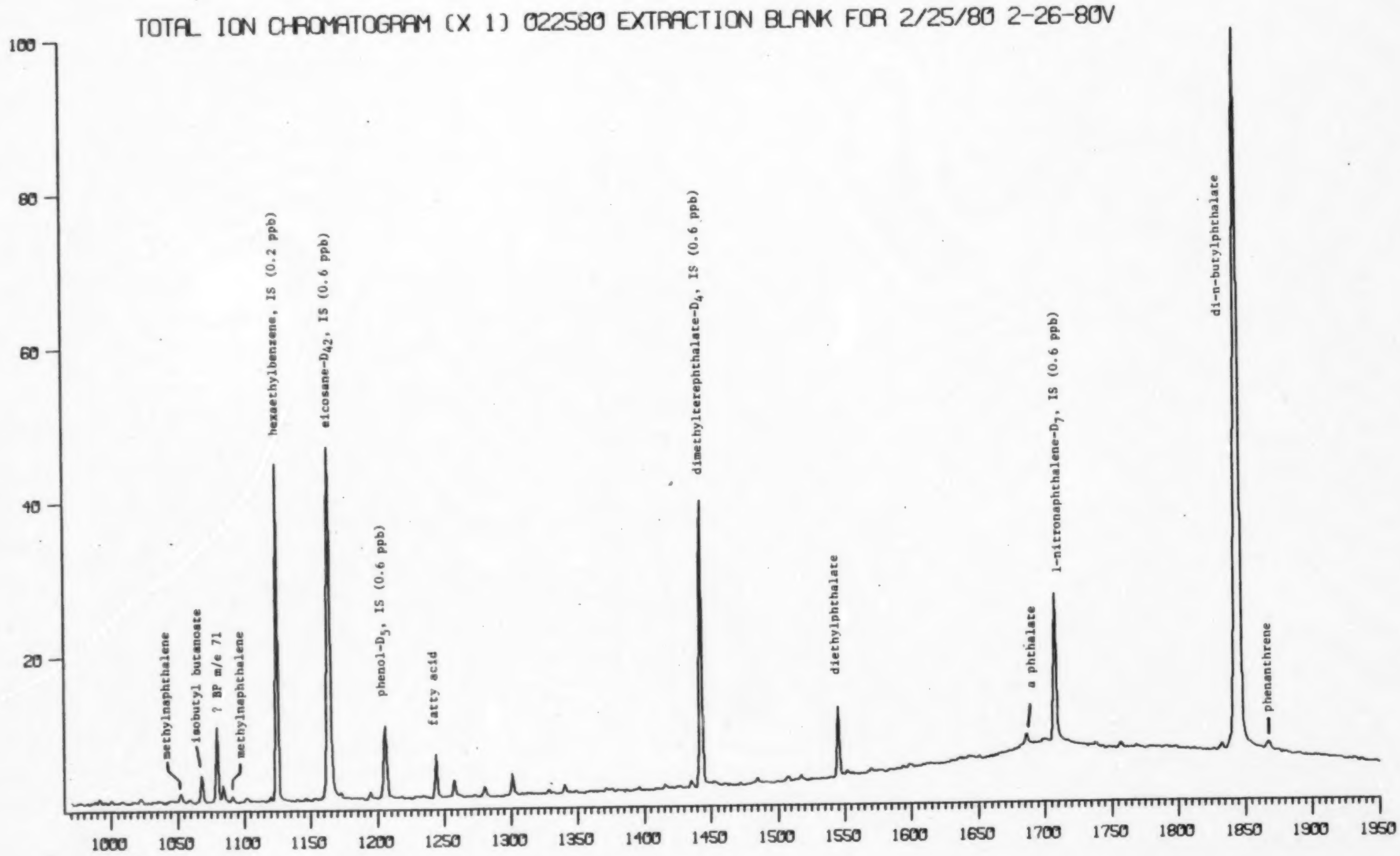

Figure 7. (continued)

computer data base was restricted to complete molecular identifications, and the Appendix D chromatograms and tables also indicate components attributable to the fractionation procedure blank, generically identified components (i.e., fatty acid, fatty alcohol, poly glycol, phthalate), and partial functional group information (i.e., the number and type of halogens present, presence of an aromatic nucleus, presence of a nitrogen atom). In addition, the main mass spectral features of significant components remaining unidentified are also presented (i.e., base peak, molecular weight and principal ions).

The analysis results of the reagent water samples S1Q and S2Q validated that the special precautions taken to minimize contamination levels for such large scale samples (10-liter) would, indeed, permit reliable detection of sample constituents at the 0.1 ppb level. The deuterated internal standards were added to the Super-Q water at the 0.6 ppb level before extraction, and the hexaethylbenzene (HEB) internal standard was added to each sample at the 0.2 ppb level (relative to the original 10-liter sample) just prior to GC-MS analysis. In one case (sample S1Q) the HEB level in the unpartitioned aliquot was 0.06 ppb. Comparison of the results of samples S1Q and S2Q with those from direct GC-MS analysis of the same amounts of internal standards showed that extraction recoveries of the deuterated internal standards ranged from 25 to 85 percent. Some of the noteworthy performance features of the S1Q and S2Q results are the following:

- Chromatograms of the unpartitioned aliquots show low levels of early eluting methylene chloride solvent impurities. The level of chloroform is an especially sensitive indicator of the effectiveness of the methylene chloride extraction solvent re-distillation.

- Di-n-butyl phthalate was the only plasticizer present at a significant level. It and the few other plasticizers found were all present at levels low enough to prevent correct identification of them in DW samples.

- The aromatic and medium polarity fraction of S1Q and S2Q showed levels of most of the background compounds to be below the part per trillion range (based on the 0.2 ppb HEB level). The somewhat higher levels of toluene and xylenes in this fraction were probably from the 4.0 ml hexane used to elute the preceding silica gel fraction.

- Most of the extraneous material in the acid fraction was found to be fatty acids, fatty alcohols and other oxygenated species some of which were probably due to the carbitol used in the diazomethane generator.

The averages for S1Q and S2Q of the net residue weight determinations for the acid, aliphatic, aromatic medium polarity and high polarity fractions were -1.9, 2.4, 1.4 and 11.2 ppb, respectively. These values are near or within the uncertainty ranges observed in each case.

Cincinnati Tap Water Samples

Samples for the second phase of the 10-liter extraction procedure method validation were Cincinnati tap water sampled at the HERL-CI laboratory. Three 1-gallon, cleaned glass jugs with Teflon-lined screw caps were filled from the tap and capped without headspace on December 10, 1979. The same volume of identical water was frozen and subjected to lyophilization which required approximately two days to reduce the volume to about one-tenth of the original. The lyophilized sample was then distributed into the 1-gallon, muffled glass jugs and filled to eliminate headspace with Super-Q reagent water. Ten-liter aliquots of these Cincinnati tap water samples (pre- and post-lyophilization, code named T3K and T3L, respectively) were extracted, concentrated, and partitioned, using the silica gel column option, as described in Section 5. Labeled chromatograms and tables of analysis results for the unpartitioned aliquot, acid and neutral fractions for samples T3L and T3K are presented in Appendix E. Inadvertently, the 10 percent aliquot for unpartitioned analysis of sample T3L was not reserved before partitioning, so corresponding analysis results are not available for that sample.

Compared to the results for the Super-Q reagent water method validation samples, discussed above, the T3K and T3L analysis results demonstrate that the 10-liter extraction method does allow the sensitive detection of a large number of organic species in relatively clean DW at the sub-ppb level. Residue weight analysis results for the T3K and T3L fractions were (μg): acid, 600 and 530; aliphatic, 0.0 and 75; aromatic/medium polarity, 30 and 87; high polarity, 150 and 500; respectively. These values are reflected in the compound identification results with relatively high %HEB values observed for compounds in the acid fractions and corresponding low ones for the neutral fraction. More than 25 percent of the identified compounds in the acid fractions for both samples had %HEB values greater than 100 with a number values greater than 500. In the neutral fractions, only 3 and 2 compounds of T3K and T3L, respectively, had %HEB values which exceeded 10 and more than half of the compounds, in both cases, had %HEB values of 2 or less.

Comparison of the identified compounds for these two data sets suggests two principal conclusions with respect to the effect of concentration of organic material in DW by lyophilization:

- Lyophilization resulted in a reduction in the levels of a number of constituents commonly identified in DW samples and concentrates.
- Lyophilization apparently introduced levels of fatty acids and some hydrocarbon species.

The first conclusion, above, is readily apparant in a comparison of the neutral (aromatic/medium polarity) fractions. The haloform, $CHBr_2Cl$, was found at a level of 65 %HEB in T3K but only 1 %HEB in T3L, and other haloforms, $CHBrCl_2$ and $CHBr_3$, were detected in T3K (7 and 2) %HEB, respectively) but not at all in T3L. Other moderately volatile compounds identified in T3K but not in T3L include the following: Two isomers of dinitrotoluene, two isomers of nitrotoluene, chlorobenzene, all three isomers of dichlorobenzene, bis-2-chloroethyl ether, phenylacetonitrile, benzonitrile and dimethoxybenzene. Comparison of the chromatograms for these two fractions (Figures E3 and E5) shows a greater amount of neutral constituents eluted earlier in the chromatogram for sample T3K than for T3L. Lower levels of recovered constituents were also seen in the results for the acid fractions with only one compound (a resin acid) of the 15 compounds found in both samples having been found at higher concentration in T3L than in T3K. The apparent loss of material accompanying lyophilization is not as pronounced for these compounds identified in the acid fraction as it was for those of the neutral fraction, as expected based on the generally lower volatility of the compounds present in the acid fraction. A further example of loss of volatile compounds upon lyophilization is presented by the results for phenol and the internal standard, phenol-D_5. The ratio of phenol to phenol-D_5 was 17:1 for T3K and 10:1 for T3L as determined by the ratios of ion intensities of corresponding ions of the native and deuterated material in the mass spectrum at the top of the phenol methyl ether GC-MS peaks. Although EICP peak area ratios were not determined in this case, the early elution of this peak (and concomitantly small degree of chromatographic separation of the deutero-analogue) as well as the large difference in the ratios, nevertheless, unambiguously illustrate the loss of volatile compounds on lyophilization.

The second conclusion, above, is also based on the identified compound results from both the acid and neutral fractions. The acid fraction contained relatively high levels of fatty acids ranging from C_8 to C_{18} including the common unsaturated C_{16} and C_{18} species. The corresponding fractionation process blank for the acid fraction contained levels of these essentially ubiquitous materials which were significantly lower than those found for T3L. However, since this family of compounds is always present in the blank to some extent, replicate sample analyses would be required to demonstrate that these fatty acids were definitely contributed by the lyophilization apparatus. The evidence for contamination of the samples by the lyophilization apparatus is more definitive in the case of the neutral fraction results. The greater proportion of late eluting material in the T3L neutral fraction chromatograms compared to that for T3K was noted above. Most of these materials were hydrocarbons with unsaturated or aromatic moieties. A possible explanation for this observation is contamination of the sample from back streaming of the pump oil in the mechanical vacuum pump of the lyophilization apparatus. This hypothesis is supported also by the residue weight results cited above wherein the aliphatic fractions contained <0.1 and 75 μg and the aromatic/medium polarity fractions contained 30 and 87 μg for T3K and T3L respectively.

The ubiquitous methylethyl maleic acid and dimethylmaleic acids were the acid fraction components found at the highest levels in T3K, but the levels of these two materials were slightly exceeded in T3L by some of the fatty acid species, cited above. Other noteworthy compounds identified in T3K and/or T3L but not mentioned in the foregoing discussion include: ethosuximide, clofibric acid, salicylic acid, m-chlorobenzoic acid, phenyl acetic acid, phenoxyacetic acid, toluic acid (all three isomers), cresol (all three isomers), dichloroacetic acid, levulinic acid, and a number of methyl and methoxy substituted benzoic acids.

SAMPLES FOR MONITORING RO PRE-CONCENTRATION OF DW AT JEFFERSON PARRISH, LOUISIANA, AND POPLARVILLE, MISSISSIPPI

Some of the sampling details of the GSRI procedure for the RO preconcentration monitoring of the two subject sites are presented in Section 4. Each of these two sampling sites were designed to reveal different aspects concerning the performance of RO pre-concentration step used to prepare the large volume DW and AWT concentrates (Volume 1). Since the Jefferson Parrish (New Orleans, Louisiana) DW was known to contain a wide variety of organic substances at levels well within the limits of the analysis method used here, the analysis results could be expected to reveal how well different classes of compounds were retained by the RO membrane processing units and also to suggest whether adsorption onto membrane surfaces significantly reduced the amounts or types of recovered species. In contrast, the Poplarville, Mississippi sampling was intended to reveal the types and levels of species introduced as artifacts to the concentrate by the RO processing apparatus since this DW source was known to be extraordinarily organic-free.

Unfortunately, none of the data obtained from analysis of these two groups of samples were useable for the above stated purposes since all of the samples were grossly contaminated by XAD-2 resin bleed artifacts. All nine of the Jefferson Parrish samples were processed through the analytical scheme (Figure 4) and analyzed by GC-MS. Although the contaminated nature of the samples was correctly assessed relatively early in the sequence for the Jefferson Parrish samples, the analyses were, nevertheless, completed in the hopes that some useful data would result. However, the only valuable result from these analyses was to provide a well-documented and definitive example of the nature of XAD-2 resin bleed artifact material. Because of the highly redundant nature of the analysis results, they were not entered in the computer data base, and only one such set of typical data are presented here. The Poplarville samples were so badly contaminated that the artifact material exceeded its solubility in the 2 to 4 ml of evaporated diethyl ether solvent. Eight of the nine Poplarville samples were analyzed as the unpartioned sample by glass capillary GC-FID to confirm their identical nature with respect to the presence of XAD-2 resin bleed contamination, and those 8 samples were not processed further. The ninth sample was found to consist of Na_2SO_4 crystals in equilibrium with a small (about 10 percent) aqueous liquid phase.

As an example of these contaminated samples, labeled GC-MS chromatograms are shown in Figures 8 and 9. These GC-MS chromatograms are for the 10-fold brine representing 50 liters of sampled DW and produced by the cellulose acetate RO membrane. This sample was concentrated on XAD-2 at acidic pH. A table which correlates with each chromatogram and lists the identified compounds follows each chromatogram (Tables 10 and 11 for the acid and neutral fractions, respectively). These results are presented to provide documentation of the types and amounts of chemical species which can be attributed to XAD-2 resin bleed. While it is possible that much of the specific detail of these results are a function of the batch of XAD-2 resin, experience with large volume DW concentrates (Volume 1) prepared by XAD-2 extraction of RO brine indicated that certain types of species, which are related to the styrene/divinyl benzene formulation of this resin, are probably independent of the resin batch. These high confidence resin

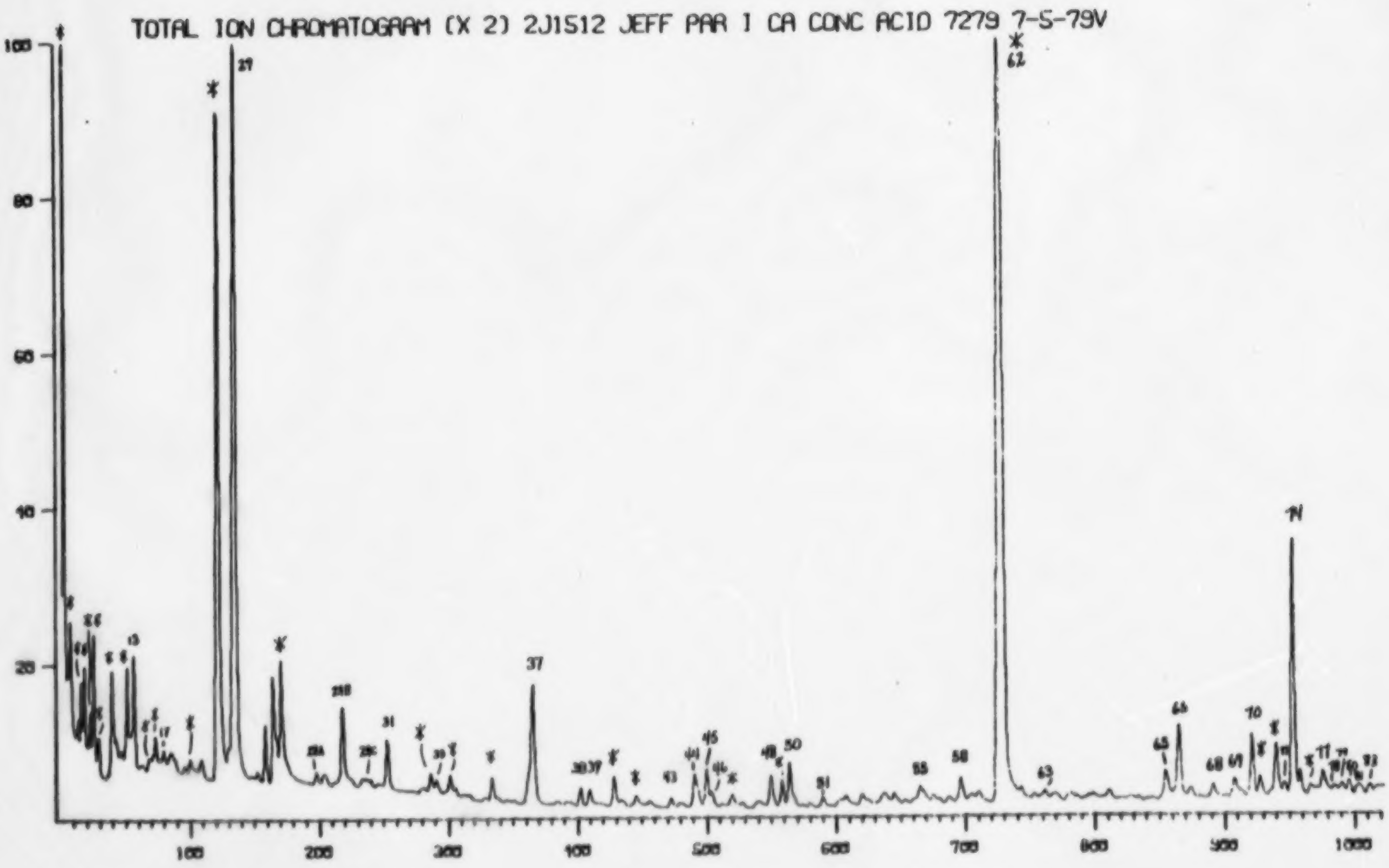

Figure 8. Residue weight analysis results for unpartitioned extracts and fractions; Cincinnati GAC Contactor D.

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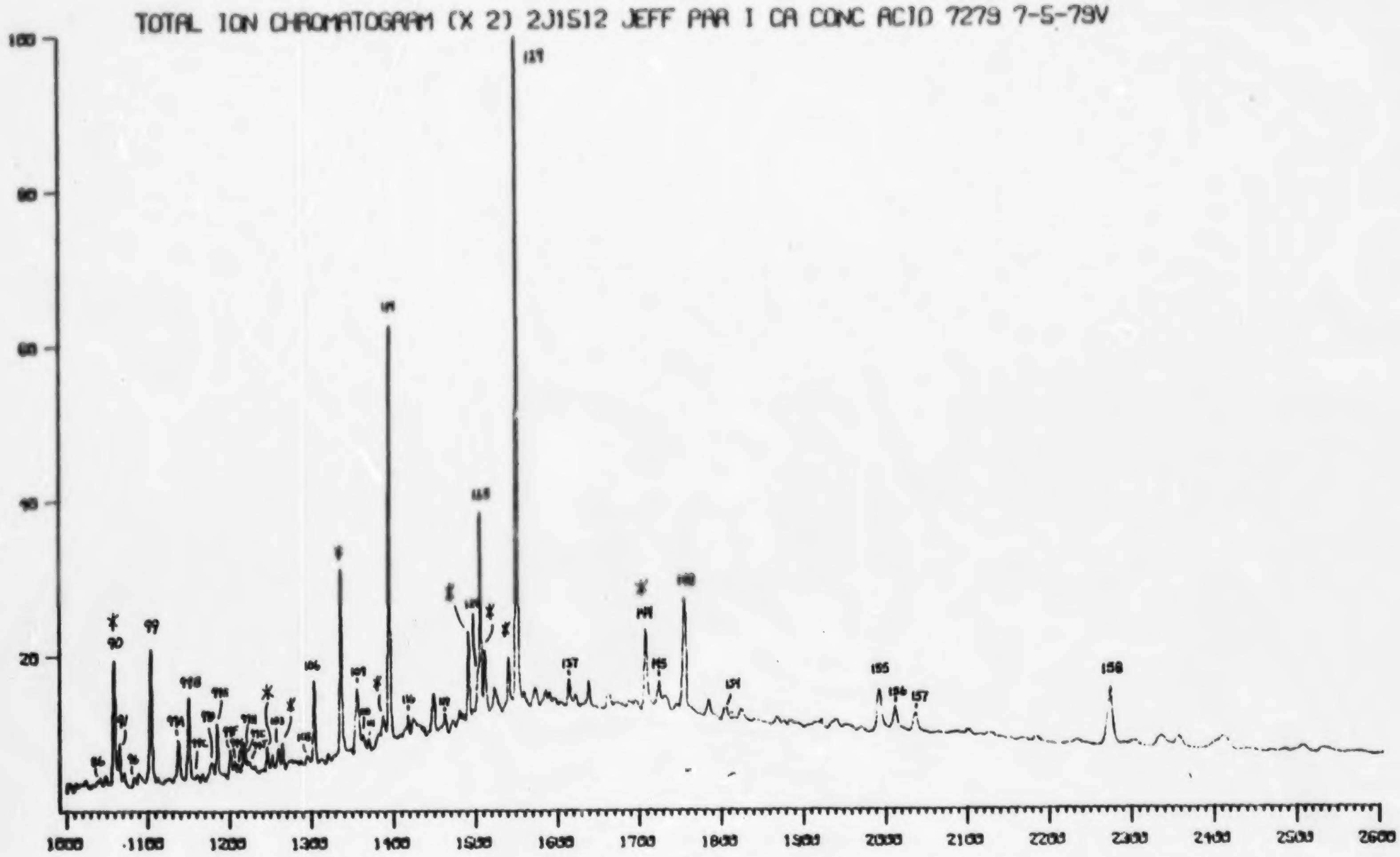

Figure 8. (Continued)

TABLE 10. GC-MS ANALYSIS RESULTS OF THE ACID FRACTION FOR THE JEFFERSON PARRISH 10-FOLD CELLULOSE ACETATE RO CONCENTRATE, ACIDIC XAD-2 EXTRACTION

Sequence[a]	Spectrum Number	RT	RRT	Compound Name[b]	Molecular Formula	Molecular Weight	Size[c]	Match[d]	Proof[e]
13	56-60	12.098	0.191	dioxane	C4.H8.O2	88	4	979	C
17	79-76	13.460	0.213	methyl dihydrofuran	C5.H8.O	84	3	920	C
29	136-140	16.525	0.261	butanol	C4.H10.O	74	6	965	B
29A	197-194	19.572	0.309	alpha-hydroxyisobutyric acid, ME	C4.H8.O3	104	3	957	C
29B	218-212	20.620	0.326	2-ethoxyethanol	C4.H10.O2	90	4	972	C
29C	237-229	21.557	0.340	methyl hexenone	C7.H12.O	112	2	956	C
31	252-249	22.302	0.352	2-ethylcaproic acid, ME	C8.H16.O2	144	4	980	A
33	291-295	24.233	0.383	heptanoic acid, ME	C7.H14.O2	130	2	964	A
37	365-356	27.893	0.440	phenol - D5, IS plus phenol - D0, ME; 7:1	C6.H6.O	94	5		A
38	402-398	29.710	0.469	dichloroacetic acid, ME	C2.H2.O2.CL2	128	3	976	A
39	409-406	30.053	0.475	1,1'-oxybis[2-ethoxy-ethane]	C8.H18.O3	162	3	919	D
43	472-469	33.153	0.523	a fatty acid, ME			2		
44	490-485	34.043	0.538	3-ethyl styrene	C10.H12	132	3	980	B
45	500-496	34.550	0.546	m-cresol, ME	C7.H8.O	108	3	997	A
46	504-509	34.753	0.549	4-ethyl styrene	C10.H17	132	2	987	A
48	549-545	36.995	0.584	dichlorobutenoic acid, ME	C4.H4.O2.CL2	154	3	man	C
50	564-561	37.758	0.596	nonanoic acid, ME; partially in blank	C9.H18.O2	158	4	975	A
51	589-586	39.002	0.616	2-methoxy-4-methylpentenoic acid	C7.H12.O3	144	2	981	C
55	665-661	42.808	0.676	delta-ketovaleric acid, ME	C5.H8.O3	116	3	916	C
58	696-692	44.387	0.701	capric acid, ME	C10.H20.O2	172	3		A
62	730-734	46.123	0.728	benzoic acid, ME - D0 + D5, IS; 12:1	C7.H6.O2	122	6	996	A
63	762-765	47.787	0.755	5-methyl-4-ketocaproic acid	C7.H12.O3	144	2	983	C
65	855-858	52.597	0.830	2,2-dimethylbutyric acid, ME	C6.H12.O2	116	3	939	D
66	865-861	53.128	0.839	naphthalene	C10.H8	128	4	984	A
68	891-886	54.497	0.860	phenylacetic acid, ME	C8.H8.O2	136	3	992	A
69	908-902	55.395	0.875	salicylic acid, ME	C7.H6.O3	138	3	980	A
70	921-917	56.087	0.886	dimethylmaleic acid, di-ME	C6.H8.O4	144	4	man	A
73	946-944	57.427	0.907	2,4,6-trichlorophenol, ME	C6.H3.O.CL3	196	2	956	A
74	953-949	57.810	0.913	2-ethyl-3-methylmaliec acid, di-ME	C7.H10.O4	158	5	989	B
77	976-972	59.063	0.933	3,5-dimethyl-benzoic acid, ME	C9.H10.O2	150	3	976	A
78	983-987	59.442	0.939	hydrocinnamic acid, ME	C9.H10.O2	150	2	902	A
79	990-987	59.822	0.945	2-methoxy-3,5,5-trimethyl-2-cyclohexene-1,4-dione	C10.H14.O3	182	2	983	B
80	996-999	60.145	0.950	3-hydroxy myristic acid, ME	C14.H28.O3	244	3	940	C
81	1003-999	60.522	0.956	2,3-dimethylbenzoic acid, ME	C9.H10.O2	150	2	905	

(continued)

TABLE 10. (continued)

Sequence[a]	Spectrum Number	RT	RRT	Compound Name[b]	Molecular Formula	Molecular Weight	Size[c]	Match[d]	Proof[e]
83	1012-1009	61.008	0.963	benzyl alcohol	C7.H8.O	108	2	990	A
86	1037-1040	62.372	0.985	6-methyl salicylic acid, ME	C8.H8.O3	166	1	933	C
90	1059-1055	63.598	1.001	hexaethylbenzene, IS					
91	1066-1063	63.997	1.007	o-chlorobenzoic acid, ME	C7.H5.O2.CL	156	3	955	A
96	1083-1080	64.937	1.022	a tetramethyl catechol isomer	C10.H14.O2	166	2	858	C
99	1104-1098	66.110	1.041	BP 113; m/e 169, 139, 95			5		
99A	1137-1130	67.948	1.070	phenol - D0 + D5, IS; 1:12	C6.H6.O	94	4	963	A
99B	1149-1143	68.620	1.080	myristic acid, ME	C14.H28.O2	228	4	986	A
99C	1160-1156	69.240	1.090	2-hydroxy benzaldehyde	C7.H6.O2	122	2	964	B
99D	1179-1170	70.308	1.107	phenoxyacetic acid, ME	C8.H8.O3	152	3	983	A
99E	1184-1181	70.592	1.111	1,1-diphenyl ethane	C14.H14	182	4	955	A
99F	1201-1197	71.555	1.127	o-salicylic acid, ME, ME	C7.H6.O3	138	3	910	C
99G	1206-1204	71.838	1.131	3-hydroxycapric acid, ME	C10.H20.O3	188	2	man	A
99H	1210-1208	72.067	1.135	p-cresol	C7.H8.O	108	2	985	A
99I	1217-1213	72.468	1.141	m-cresol	C7.H8.O	108	3	983	A
99J	1224-1228	72.872	1.147	p-hydroxybenzoic acid, ME, ME	C7.H6.O3	138	2		A
103	1259-1256	74.883	1.179	clofibric acid, ME	C10.H11.O3.CL	214	3	977	B
105	1294-1291	76.910	1.211	ethylbiphenyl	C14.H14	182	2	922	C
106	1303-1299	77.437	1.219	a diethylbiphenyl isomer	C16.H18	210	4	848	C
109	1355-1350	80.498	1.268	a diethylbiphenyl isomer	C16.H18	210	4	850	C
110	1364-1367	81.038	1.276	dichlorosalicylic acid, ME	C7.H4.O3.CL2	206	2	889	B
111	1369-1372	81.337	1.281	a phthalate			2		
114	1395-1390	82.888	1.306	phthalic acid, di-ME	C8.H6.O4	166	6	980	A
116	1423-1420	84.580	1.332	phthalate, methyl ethyl					
119	1462-1467	86.940	1.369	3,4-dihydroxy benzaldehyde, di-ME	C7.H6.O3	138	3	964	B
124	1502-1499	89.397	1.408	3,4-dihydroxybenzoic acid, tri-ME	C7.H6.O4	154	3	972	B
125	1506-1499	89.643	1.412	BP 153; m/e 59, 125, 152, 169, 180, 184, 212		212?	5		
129	1548-1545	92.248	1.453	monobutylphthalate, ME	C12.H14.O4	222	6	944	A
137	1614-1609	96.372	1.518	4-hydroxy-xanthen-9-one	C13.H8.O3	212	3	802	C
144	1708-1703	102.282	1.612	di-n-butylphthalate, partially in blank	C16.H22.O4	278	4	987	A
145	1724-1718	103.287	1.628	a trimethyl dihydronaphthalenone	C13.H16.O	188	3	870	C
148	1745-1741	104.608	1.648	3,4-dihydroxycinnamic acid, tri-ME	C9.H8.O4	166	2	803	C
154	1804-1799	108.318	1.707	a methyl alkylphthalate			3		

(continued)

TABLE 10. (continued)

Sequence[a]	Spectrum Number	RT	RRT	Compound Name[b]	Molecular Formula	Molecular Weight	Size[c]	Match[d]	Proof[e]
155	1993-1985	120.245	1.895	BP 193; m/e 210, 179		266?	4		
156	2012-2005	121.453	1.914	isomer of #155			3		
157	2036-2027	122.983	1.939	similar to #156			3		
158	2274-2262	138.033	2.173	dehydroabietic acid, ME	C20.H28.O2	300	4	992	B

a) The sequence number is used to label the peaks in the GC-MS chromatogram, Figure 8.

b) ME = methyl ester or methyl ether; IS = internal standard.

c) Size (height) of the GC peak in the GC-MS chromatogram (see a, above) related to the internal standard, hexaethyl benzene. The RS (relative size) parameter is explained in Section 5.

d) The quality index of the computer mass spectral library match (Finnigan INCOS software) where the value 1000 reflects a perfect fit of the data mass spectrum with the library mass spectrum.

e) Proof reflects the confidence level of the analyst: A, confirmed identification by comparison to data from a standard; B, highest confidence level for non-confirmable compounds; C, less than 80% confidence level; D, less than 50% confidence level.

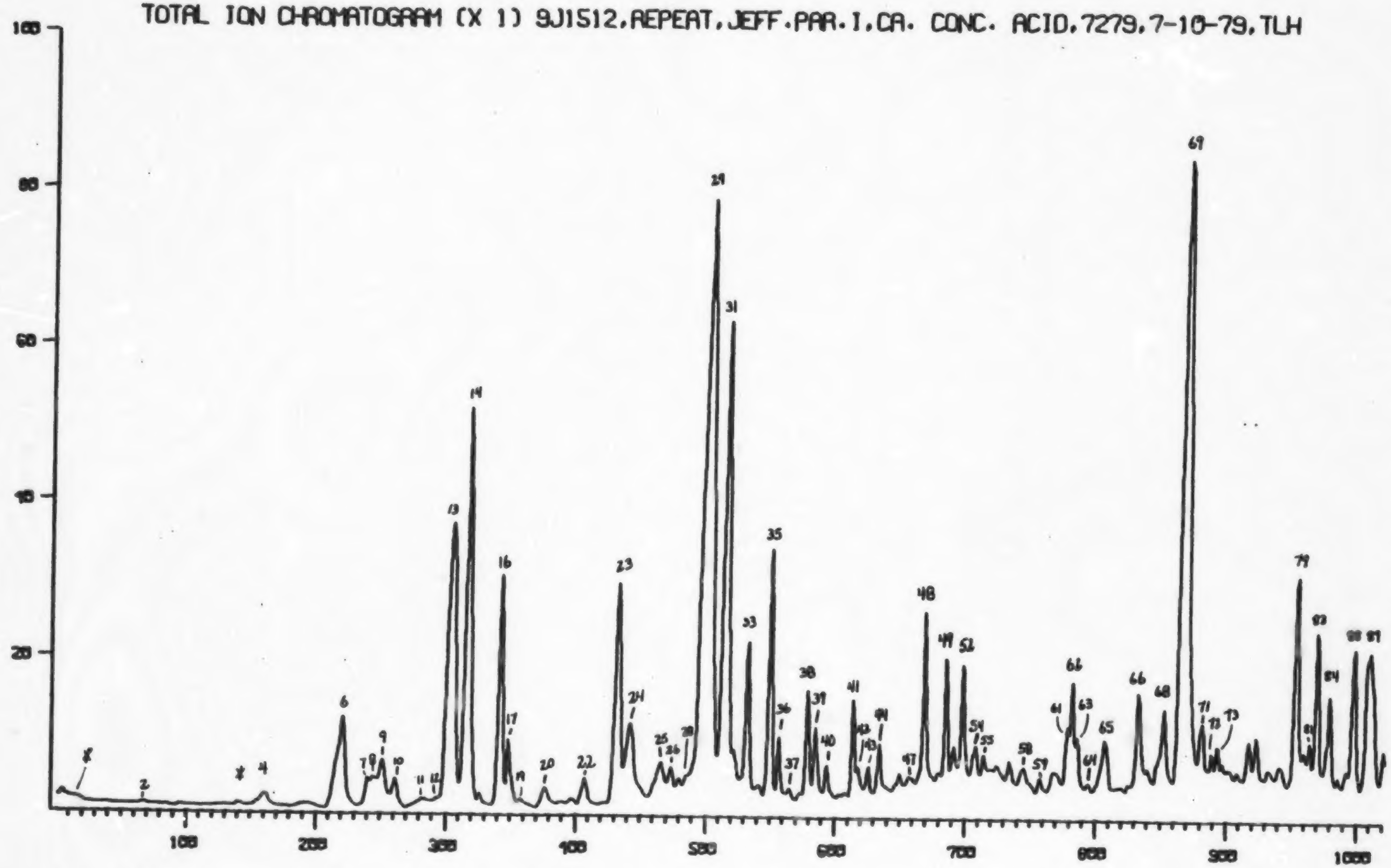

Figure 9. Compound identification results for the seven samples associated with Cincinnati GAC Contactor D.

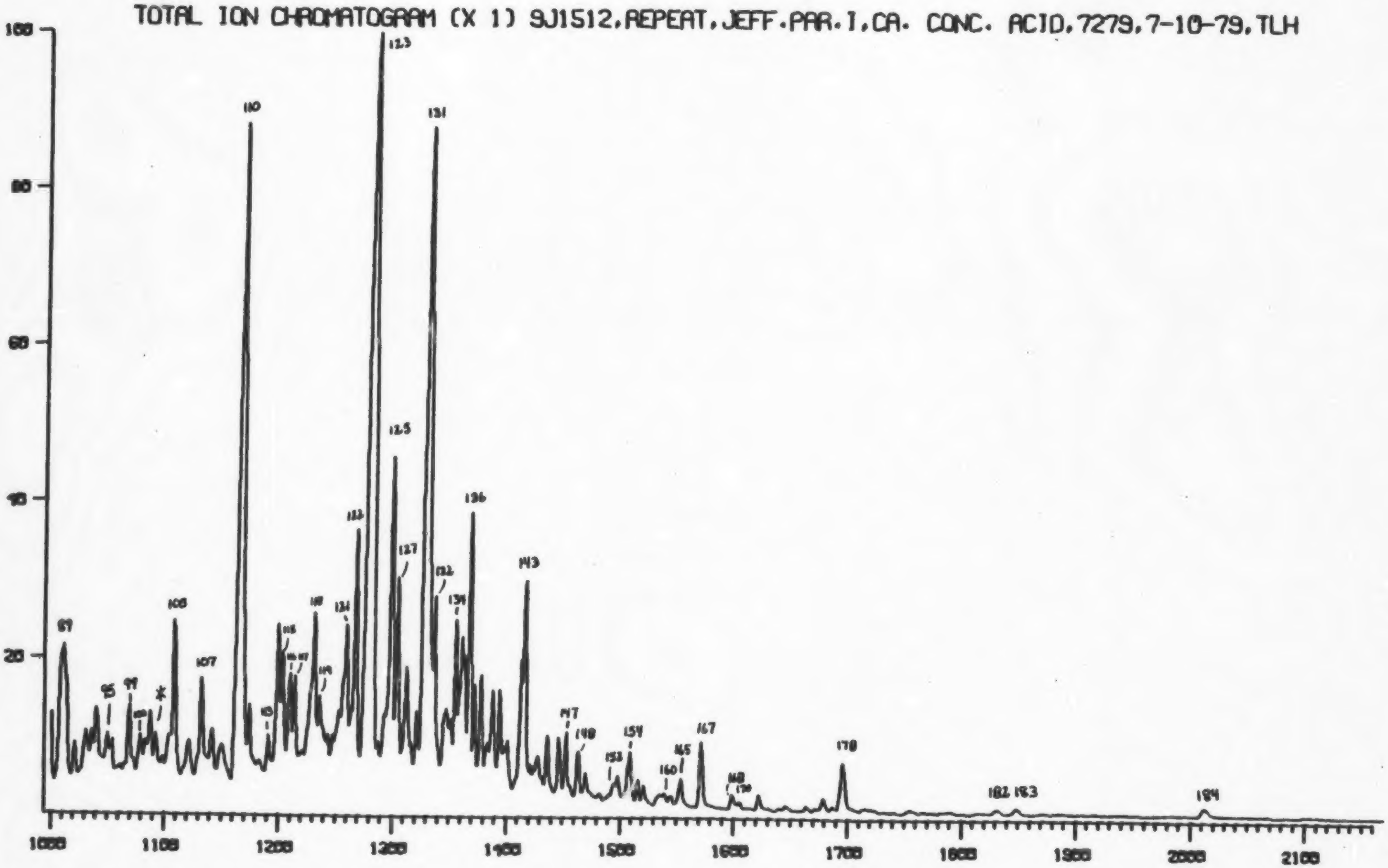

Figure 9. (Continued)

TABLE 11. GC-MS ANALYSIS RESULTS OF THE AROMATIC/MEDIUM POLARITY FRACTION FOR THE JEFFERSON PARRISH 10-FOLD CELLULOSE ACETATE RO CONCENTRATE, ACIDIC XAD-2 EXTRACTION

Sequence[a]	Spectrum Number	RT	RRT	Compound Name[b]	Molecular Formula	Molecular Weight	Size[c]	Match[d]	Proof[e]
2	66-61	11.133	0.163	p-xylene	C8.H10	106	3	991	A
4	160-148	16.542	0.242	1,3-dimethyladamantane	C12.H20	164	4	man	A
6	220-207	19.942	0.292	a dimethyldecalin isomer	C12.H22	166	6	971	B
7	240-234	21.078	0.308	styrene	C8.H8	104	4	960	B
8	245-235	21.362	0.313	a dimethyldecalin isomer	C12.H22	166	3	977	B
9	252-257	21.760	0.318	" " "	C12.H22	166	5	985	B
10	261-268	22.270	0.326	" " "	C12.H22	166	4	986	B
11	282-270	23.458	0.343	similar to #4			4		
12	294-289	24.138	0.353	similar to #4			3		
13	300-295	24.480	0.358	m-diethylbenzene	C10.H14	134	7	980	A
14	314-311	25.258	0.370	p-diethylbenzene	C10.H14	134	7	956	A
16	341-334	26.793	0.392	o-diethylbenzene	C10.H14	134	6	957	A
17	348-346	27.190	0.398	an ethyl isopropylbenzene isomer	C11.H16	148	5	987	B
19	357-368	27.702	0.405	bromobenzene - D5, IS					
20	376-370	28.778	0.421	an isopropylethylbenzene isomer	C11.H16	148	4	973	B
22	407-401	30.553	0.447	a dimethylpropylbenzene isomer	C11.H16	148	5	950	C
23	431-425	31.927	0.467	2-ethyl styrene	C10.H12	132	6	935	B
24	442-437	32.558	0.476	a methyl pentylbenzene isomer	C12.H18	162	5	865	C
25	466-455	33.948	0.497	a methyl allyl benzene isomer	C10.H12	132	5	968	B
26	474-477	34.413	0.504	a dimethylbutylbenzene isomer	C12.H18	162	4	958	C
28	486-483	35.112	0.514	p-ethylpropyltoluene	C12.H18	162	3	960	C
29	494-488	35.577	0.521	3-ethyl styrene	C10.H12	132	7	926	B
31	512-509	36.587	0.535	4-ethyl styrene	C10.H12	132	7	928	A
33	533-527	37.783	0.553	1,3,5-triethylbenzene	C12.H18	162	6	979	A
35	549-545	38.705	0.566	a methyl allyl benzene isomer	C10.H12	132	7	948	B
36	557-554	39.158	0.573	a C-6 benzene	C12.H18	162	5		
37	565-569	39.623	0.580	a methyl allyl benzene isomer	C10.H12	132	4	951	C
38	579-575	40.432	0.592	1,2,4-triethylbenzene	C12.H18	162	6	994	A
39	585-582	40.778	0.597	a dimethyl allyl benzene isomer	C11.H14	146	5	951	B
40	594-590	41.302	0.604	a methyl allyl benzene isomer	C10.H12	132	5	985	B
41	614-1195	42.462	0.621	tetralin	C10.H12	132	6	985	A
42	618-622	42.693	0.625	methyltetralin	C11.H14	146	4	957	B
43	625-622	43.102	0.631	an (ethylpropyl)propylbenzene isomer	C14.H22	190	5	945	B
44	634-630	43.628	0.638	C8 - benzene	C14.H22	190	5		

(continued)

TABLE 11. (continued)

Sequence[a]	Spectrum Number	RT	RRT	Compound Name[b]	Molecular Formula	Molecular Weight	Size[c]	Match[d]	Proof[e]
47	657-653	44.968	0.658	a methyltetralin isomer	C11.H14	146	3	978	B
48	669-664	45.668	0.668	divinylbenzene	C10.H10	130	6	931	B
49	685-680	46.603	0.682	a methyl indene isomer	C10.H10	130	6	989	B
52	698-695	47.365	0.693	BP 117; MW 146; aromatic			6		
54	708-712	47.952	0.702	a dimethyl indan isomer	C11.H14	146	5	931	B
55	715-711	48.368	0.708	cycloprop[A]tetrahydroindene	C10.H10	130	4	982	B
58	745-739	50.145	0.734	trimethylbenzaldehyde	C10.H12.O	148	4	948	B
59	757-754	50.855	0.744	heptenylbenzene	C13.H18	174	4	971	B
61	779-774	52.165	0.763	a tetraethylbenzene isomer	C14.H22	190	5	976	B
62	783-780	52.402	0.767	a tetraethylbenzene isomer	C14.H22	190	4	974	C
63	786-791	52.582	0.769	cyclohexylbenzene	C12.H16	160	3	992	A
64	795-798	53.120	0.777	an ethyl tetralin isomer	C12.H16	160	3	907	C
65	808-798	53.893	0.789	an ethyl tetralin isomer	C12.H16	160	6	967	B
66	833-827	55.388	0.811	BP 91; m/e 104, 119, 131, 174, 190; a styrene oligomer			6		
68	853-857	56.590	0.828	an ethyl tetralin isomer	C12.H16	160	6	978	B
69	873-878	57.772	0.845	naphthalene	C10.H8	128	7	857	A
71	881-877	58.255	0.853	a C-3 tetralin					
72	889-886	58.738	0.860	an ethyl tetralin isomer	C12.H16	160	5	988	B
73	894-891	59.040	0.864	a trimethyl dehydronaphthaleneone	C13.H16.O	188	4	850	C
79	954-948	62.687	0.917	dihydrodimethylindene-4-carboxylic acid ethyl ester	C14.H18.O2	218	6	932	C
81	964-962	63.298	0.926	octenyl benzene	C14.H20	188	5	907	C
83	970-967	63.663	0.932	BP 117; m/e 91, 132, 145, 159, 188; an alkyl tetralin			6		
84	979-974	64.215	0.940	2-methylnaphthalene	C11.[illegible]0	142	6	961	A
88	998-993	65.382	0.957	similar to #83			6		
89	1010-1003	66.117	0.968	trimethyl dihydronaphthalenone , mixture	C13.H16.O	188	6	862	C
95	1049-1046	68.517	1.000	hexaethylbenzene, IS					
99	1069-1065	69.750	1.018	2-ethylnaphthalene	C12.H12	156	5	987	A
100	1079-1075	70.368	1.027	1-ethylnaphthalene	C12.H12	156	5	957	A
105	1108-1114	72.167	1.053	biphenyl	C12.H10	154	6	903	A
107	1132-1125	73.652	1.075	diphenylmethane	C12.H12	168	6	974	A
110	1161-1158	75.447	1.101	1,1-diphenyl ethane	C14.H14	182	7	949	A
113	1191-1187	77.283	1.128	octahydrophenanthrene, mixture	C14.H18	186	5	932	D
115	1204-1207	78.083	1.140	a methylbiphenyl isomer, mixture	C13.H12	168	6	927	C

(continued)

TABLE 11. (continued)

Sequence[a]	Spectrum Number	RT	RRT	Compound Name[b]	Molecular Formula	Molecular Weight	Size[c]	Match[d]	Proof[e]
116	1209-1206	78.393	1.145	bibenzyl	C14.H14	182	5	933	A
117	1214-1218	78.703	1.149	a methyl biphenyl isomer	C13.H12	168	5	976	C
118	1231-1221	79.755	1.164	BP 91; m/e 104, 117, 131, 146, 242; a styrene oligomer			6		
119	1236-1234	80.068	1.169	1,1-diphenylethylene, mixture	C14.H12	180	5	902	C
121	1259-1247	81.493	1.190	similar to #118			6		
122	1268-1265	82.045	1.198	BP 168; a diphenylmethane analogue			7		
123	1275-1271	82.478	1.204	a diethyl biphenyl isomer	C16.H18	210	8	860	B
125	1297-1289	83.818	1.224	BP 104; m/e 91, 117, 138, 200, 214, 242; a styrene oligomer			7		
127	1304-1302	84.250	1.230	similar to #122 plus m/e 133			6		
131	1325-1323	85.558	1.249	BP 195; m/e 105, 165, 181, 210, 223, 238			7		
132	1337-1340	86.283	1.260	a dimethylbenzophenone isomer	C15.H14.O	210	6	860	C
134	1355-1353	87.415	1.277	a di(ethylphenyl)ethane isomer	C18.H22	238	6	968	B
136	1367-1365	88.168	1.288	a di(ethylphenyl)ethane isomer	C18.H22	238	6	967	B
143	1417-1421	91.327	1.334	di(C-2 phenyl) ethane	C18.H22	238	6	974	B
147	1453-1450	93.612	1.367	1-phenyltetralin	C16.H16	208	5	986	B
148	1463-1459	94.247	1.377	di(C-2 phenyl)ethane	C18.H22	238	5	974	B
152	1494-1487	96.208	1.405	tetrahydrodibenzo cyclooctene	C16.H16	208	3	930	C
154	1509-1502	97.152	1.419	stilbene	C14.H12	180	5	972	A
160	1539-1542	99.023	1.446	1-phenyl 3,4-dihydronaphthalene	C16.H14	206	3	968	A
165	1554-1548	99.955	1.460	1-nitronaphthalene - D7, IS					
167	1571-1577	101.002	1.475	2-phenyltetralin	C16.H16	208	5	991	B
168	1599-1595	102.718	1.501	a dimethylfluorine isomer	C15.H14	194		940	C
170	1605-1610	103.080	1.506	a dimethylfluorine isomer	C15.H14	194	4	953	C
178	1696-1690	108.583	1.586	phenanthrene	C14.H10	178	5	969	A
182	1831-1824	116.608	1.704	2-methylphenanthrene	C15.H12	192	3	976	B
183	1848-1842	117.608	1.718	1-methylanthracene	C15.H12	192	3	977	B
184	2013-2002	127.212	1.859	2-phenylnaphthalene	C16.H12	204	4	978	A

a) The sequence number is used to label the peaks in the GC-MS chromatogram, Figure 9.

b) ME = methyl ester or methyl ether; IS = internal standard.

c) Size (height) of the GC peak in the GC-MS chromatogram (see a, above) related to the internal standard, hexaethyl benzene. The RS (relative size) parameter is explained in Section 5.

d) The quality index of the computer mass spectral library match (Finnigan INCOS software) where the value 1000 reflects a perfect fit of the data mass spectrum with the library mass spectrum.

e) Proof reflects the confidence level of the analyst: A, confirmed identification by comparison to data from a standard; B, highest confidence level for non-confirmable compounds; C, less than 80% confidence level; D, less than 50% confidence level.

bleed indicators are styrene and divinylbenzene (trivally), the ethyl styrene isomers, other compounds containing the ethylphenyl or vinylphenyl moiety and bisphenyl compounds (for example, diphenyl ethanes). In addition, large amounts of benzaldehyde and benzoic acid, plus smaller amounts of alkylated analogues, probably are from oxidation of the vinylphenyl moiety. Other compounds which are not clearly related chemically to the resin formulation are numerous partially reduced alkylated naphthalenes, indenes, and indans; unsubstituted and methylated polynuclear aromatic hydrocarbons (usually not larger than phenanthene) are also nearly always found at low levels with a few partially reduced species present. These species which do not contain the phenyl group may arise from hydrocarbon solvent used at some stage of XAD-2 resin manufacturing. All of the compounds found in the aromatic/medium polarity fraction (Figure 9 and Table 11) are qualified for classification as XAD-2 resin bleed artifacts on the basis of the above criteria. Except for the substituted benzoic acids, noted above, a similarly definitive classification of species in the acid fraction that are resin artifacts cannot be proposed at this time. Note, however, that many of the neutral constituents present at highest levels in the aromatic/medium polarity fraction are also present at low levels in the acid fraction due to carry-through from the very high levels present. Typically, the ratio of material recovered in the acid and aromatic/medium polarity fractions for these Jefferson Parrish samples was about 1:2, acid:aromatic/medium polarity. For comparison, typical ratios for these fractions in samples not containing XAD-2 artifacts were in the range 3:1 to 50:1 (see, for example, Tables 4 and 8 and Tables 7 and 8 of Volume 1).

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APPENDIX A

THE 6-DIGIT CODE USED FOR SMALL-VOLUME WATER SAMPLES AND THEIR FRACTIONS

The following describes a 6-digit code which was used for the data system file name for each GC-MS analysis of the four sets of small-volume samples. A similar but more elaborate 6-digit code system was also used for the large-volume organic concentrates; it can be found in Volume 1 of this report. Knowledge of this code is not necessary for the understanding of this report; however, the code does appear in the computer-printed tables and other analysis results in appendices of this volume.

1. Digit One: A number corresponding to the partitioned fraction.

    0 = Unprocessed extract or concentrate, as received
    2 = Acid Fraction (derivatized)
    3 = 2.75 ml hexane eluate from silica gel (not analyzed by GC-MS)
    4 = Neutral compounds (no acids or bases); no other fractionation
    9 = 4 ml elution of silica gel with methylene chloride following Fraction 3, above.

2. Digit 2: A letter indicating the origin of the water sample.

    T = Cincinnati, Ohio
    J = Jefferson Parish, (New Orleans) Louisiana
    S = A "Super-Q" water blank

3. Digit Three: Numbers 1 to 6 (sampling sequence of the site)

4. Digit Four: A letter corresponding to the method of extraction of organic material from the original water or a number indicating the sampling point from the RO process (Jefferson Parrish only)

    Letters indicate:

    Y = XAD extraction of the water directly with diethyl ether elution
    E = Water sampled before GAC contactor treatment
    G = Water sampled after GAC contactor treatment
    R = Water which has been concentrated by reverse osmosis; either before or after GAC contactor treatment
    Q = A "Super-Q" water blank
    L = A sample concentrated by lyophylization
    K = A sample without treatment corresponding to that concentrated by lyophylization

Numbers indicate:

XAD analytical samples for the Jefferson Parrish sampling. These were generated from reverse osmosis concentration process monitoring and are coded as follows:

Stage of RO Processing	Code Number pH of Sample Acidic	 Basic
Cellulose Acetate Feed	1	2
Cellulose Acetate Permeate (Nylon Feed)	3	4
Cellulose Acetate Concentrate	5	6
Nylon Concentrate	7	8

The number 9 in the third digit indicates the sample is a blank XAD elution.

5. Digit Five:

   1. For GAC contactor A and D related samples, this digit is a running index and has no other assigned meaning. Reference the sampling flow diagram in each case (Figures 2 and 3).

   2. For other samples (except large-volume organic concentrates) this digit is a 1 and carries no meaning.

6. Digit Six: A number corresponding to whether the data file corresponds to the first, second, etc., time GC-MS analysis of the sample has been performed.

Thus, an example would be:

9T4G32

This file name would indicate that it was the second attempt to analyze the methylene chloride eluted silica gel fraction of a sample produced from the fourth sampling of Cincinnati drinking water after processing by a GAC contactor. In addition, this is the third sample produced from that water.

APPENDIX B

COMPOUND IDENTIFICATION RESULTS FOR THE THIRTEEN CINCINNATI GAC CONTACTOR A SAMPLES--COMPUTER-PRINTED TABLES

Appendix B contains the compound identification results for the thirteen Cincinnati GAC contactor A samples as the separate computer-printed tables for each sample. These individual listings are in decreasing order of the RS values of the GC peaks. Their presentation as separate lists for each sample facilitates the review of the compound identification results of individual samples compared to the use of Table 5 for that purpose. The information provided for each identified compound by these tables which is not available in the combined computer-printed listing of Table 5 includes the following:

- RS values for each identified compound
- Identification status (confirmed, P, and tentative, T) for each identified compound
- The CAS number for each identified compound
- The systematic name of each compound
- The fraction in which each identification was made (acid, aromatic/medium polarity neutrals, or unpartitioned neutrals)

Column headers and symbols used in these computer-printed tables are explained in the section, Abbreviations and Symbols.

TABLE B1. COMPOUND IDENTIFICATION RESULTS FOR THE CINCINNATI GAC CONTACTOR A SAMPLE, T4R5, PRE-GAC 100-FOLD NYLON RO BRINE

COMPOUNDS FOUND IN CONCENTRATE BY RELATIVE SIZE (PART I)
UNDER FRACTION, 1=FOUND ON GC COLUMN 1, 2=FOUND ON GC COLUMN 2, 3=FOUND ON BOTH GC COLUMN 1 AND GC COLUMN 2
CINCINNATI IV GAC FEED 100 X NYL RO

Code Name T4R5

SEQ NO.	RS	SYSTEMATIC NAME	CAS NO.	FRACTION 2	FRACTION 9	POS. OR TENT ID	CONC. (%HEB)
1	9.36	2-ETHYLHEXANOIC ACID	149575	1		P	84.00
2	9.36	%BENZOIC ACID	65850	1		P	45.00
3	9.36	3,4-DIMETHYLBENZOIC ACID	619045	1		P	60.00
4	9.36	1,2,3,4,4A,9,10,10A-OCTAHYDRO-1,4A-DIMETHYL-7-(1-METHYLETHYL)-1-PHENANTHRENEC	5155704	1		T	81.00
5	8.36	%HEPTANOIC ACID	111148	1		P	84.00
6	8.36	CIS-2-ETHYL-3-METHYL-2-BUTENEDIOIC ACID	41654095	1		T	76.00
7	8.36	(2,5-DIMETHYLBENZENE)BUTANOIC ACID	1453061	1		T	28.00
8	8.36	9-OXODECANOIC ACID	1[illegible]22260	1		T	47.00
9	7.36	2-ETHOXYPROPANE	625547	1		T	11.00
10	7.36	%NONANEDIOIC ACID	123999	1		P	15.00
11	7.36	4-(1,5-DIMETHYL-3-OXOHEXYL)CYCLOHEXANECARBOXYLIC ACI)	38963916	1		T	10.00
12	7.36	OCTAHYDRO-1,4A-DIMETHYL-1-PHENANTHRENE CARBOXILIC ACID, METHYL ESTER	3650042	1		T	11.00
13	7.36	4-METHYL-4-NITROPENTANOIC ACID	23102025	1		T	19.00
14	7.36	2-PYRROLIDONE	616455	1		P	12.00
15	7.36	CIS-2,3-DIMETHYLBUTENEDIOIC ACID	488211	1		P	22.00
16	7.36	%*+$2,4,6-TRICHLOROPHENOL	88062	1		P	10.00
17	7.36	%3,5-DICHLOROPHENOL	591355	1		T	19.00
18	7.36	5-HEXYLDIHYDROFURANONE	706149	1		T	22.00
19	6.36	%1-BUTANOL	71363	1		P	5.00
20	6.36	3-METHOXY-3-METHYL-2-BUTANONE	36687986	1		T	4.00
21	6.36	2-(4-CHLOROPHENOXY)-2-METHYLPROPANOIC ACID	882097	1		P	3.00
22	6.36	%1,2-BENZENEDICARBOXYLIC ACID	88993	1		P	4.00
23	6.36	%1,2-BENZENEDICARBOXYLIC ACID, MONOBUTYL ESTER	131704	1		P	5.00
24	6.36	1,3-DIMETHYL-2-(2-ISOPROPYLPHENYL)ETHYLCYCLOHEXANE CARBOXILIC ACID	6080	1		T	54.00
25	6.36	2-METHYL BENZOIC ACID	118901	1		P	5.00
26	6.36	ANTEISOUNDECANOIC ACID	5601505	1		T	5.00
27	6.36	3-METHYLBENZOIC ACID	99047	1		P	6.00
28	6.36	ALPHA-METHYLBENZENEACETIC ACID	492375	1		P	1.00
29	6.36	%3-PHENYLPROPIONIC ACID	501520	1		P	7.00
30	6.36	3,5-DIMETHYL BENZOIC ACID	499069	1		P	4.00
31	6.36	ACETIC ACID, 2-METHYL PHENYL ESTER	533186	1		T	3.00
32	6.36	%*+$2,4-DICHLOROPHENOL	120832	1		T	3.00
33	6.36	ANTEISOTRIDECANOIC ACID	25403145	1		T	3.00
34	6.36	ISO-TRIDECANOIC ACID	25448242	1		T	5.00
35	6.36	ISOMYRISTIC ACID	543	1		P	5.00
36	6.36	4-METHOXYBENZOIC ACID	100094	1		P	5.00

TABLE B2. COMPOUND IDENTIFICATION RESULTS FOR THE CINCINNATI GAC CONTACTOR A SAMPLE, T4R4 PRE-GAC 10-FOLD NYLON R RO BRINE

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COMPOUNDS FOUND IN CONCENTRATE BY RELATIVE SIZE (PART I)
UNDER FRACTION, 1=FOUND ON GC COLUMN 1, 2=FOUND ON GC COLUMN 2, 3=FOUND ON BOTH GC COLUMN 1 AND GC COLUMN 2
CINCINNATI IV GAC FEED 10 X NYL RO

Code Name T4R4

SEQ NO.	RS	SYSTEMATIC NAME	CAS NO.	FRACTION 2	FRACTION 9	POS. OR TENT ID	CONC. (%MEB)
1	11.36	%BENZOIC ACID	65850	1		P	25.00
2	8.36	2-ETHYLHEXANOIC ACID	149575	1		P	51.00
3	8.36	%HEPTANOIC ACID	111148	1		P	40.00
4	8.36	10-OXO-UNDECANOIC ACID	676006	1		T	34.00
5	8.36	1,3-DIMETHYL-2-(2-ISOPROPYLPHENYL)ETHYLCYCLOHEXANE CARBOXILIC ACID	6980	1		T	48.00
6	7.36	%HEXANOIC ACID	142621	1		P	25.00
7	7.36	10-UNDECENOIC ACID	112389	1		T	11.00
8	7.36	2-ETHYL-3-METHYL-2-BUTENEDIOIC ACID	2007	1		T	22.00
9	7.36	%*+$2,4-DICHLOROPHENOL	120832	1		P	13.00
10	7.36	2-ACETYL-P-TOLUIC ACID	15482549	1		T	22.00
11	7.36	9-OXODECANOIC ACID	1422260	1		T	11.00
12	7.36	OCTAHYDRO-1,4A-DIMETHYL-1-PHENANTHRENE CARBOXILIC ACID, METHYL ESTER	3650042	1		T	13.00
13	6.36	4-METHYL-2-PENTANOL	108112	1		T	4.00
14	6.36	2-PYRROLIDONE	616455	1		P	3.00
15	6.36	CIS-2,3-DIMETHYLBUTENEDIOIC ACID	488211	1		P	9.00
16	6.36	%*+$2,4,6-TRICHLOROPHENOL	88062	1		P	4.00
17	6.36	%3-PHENYLPROPIONIC ACID	501520	1		P	3.00
18	6.36	%NONANEDIOIC ACID	123999	1		P	7.00
19	6.36	ANTEISOHEPTADECANOIC ACID	457	1		P	11.00
20	6.36	HEPTADECENOIC ACID	26265996	1		T	6.00
21	6.36	%1-HEXADECANOL	36653824	1		P	12.00
22	6.36	4-(1,5-DIMETHYL-3-OXOHEXYL)CYCLOHEXANECARBOXYLIC ACID	38963916	1		T	3.00
23	6.36	2-BUTYLTETRAHYDROFURAN	1004291		1	T	5.00
24	6.36	%BROMODICHLOROMETHANE	75274		1	P	4.00
25	6.36	%DIBROMOCHLOROMETHANE	124481		1	P	6.00
26	5.36	%UNDECANOIC ACID	112378	1		P	2.00
27	5.36	ALPHA-METHYLBENZENEACETIC ACID	492375	1		P	1.00
28	5.36	3-METHYLBENZOIC ACID	99047	1		P	3.00
29	5.36	4-METHYLBENZOIC ACID	99945	1		P	2.00
30	5.36	ACETIC ACID, 2-METHYL PHENYL ESTER	533186	1		T	1.50
31	5.36	4-METHYLENE-1-(1-METHYLETHYL)CYCLOHEXENE	99843		1	T	2.00
32	5.36	1-HEXANOL	111273		1	P	1.00
33	5.36	%TRIBROMOMETHANE	75252		1	P	3.00
34	5.36	%*+$1,4-DICHLOROBENZENE	106467		1	P	0.50
35	5.36	%+$1,2-DICHLORO BENZENE	95501		1	P	2.00
36	5.36	O-NITROTOLUENE	88722		1	T	2.00
37	5.36	%BENZENEACETONITRILE	140294		1	P	1.00
38	5.36	1,3-DIMETHYLNAPHTHALENE	575417		1	T	2.00
39	5.36	1-(2-PROPENYL)NAPHTHALENE	2489863		1	T	2.00
40	5.36	TRIMETHYLNAPHTHALENE	317		1	T	1.50
41	5.36	TRIMETHYLNAPHTHALENE	311		1	T	0.50
42	5.36	2,6-DINITROTOLUENE	606202		1	P	2.00
43	5.36	%1-METHYL-2,4-DINITROBENZENE	121142		1	P	2.00

TABLE B3. COMPOUND IDENTIFICATION RESULTS FOR THE CINCINNATI GAC CONTACTOR A SAMPLE, T4R3, PRE-GAC CELLULOSE ACETATE RO PERMEATE

COMPOUNDS FOUND IN CONCENTRATE BY RELATIVE SIZE (PART I)
UNDER FRACTION, 1=FOUND ON GC COLUMN 1, 2=FOUND ON GC COLUMN 2, 3=FOUND ON BOTH GC COLUMN 1 AND GC COLUMN 2
CINCINNATI IV GAC FEED CA PERMEATE

Code Name T4R3

SEQ NO.	RS	SYSTEMATIC NAME	CAS NO.	FRACTION 2	FRACTION 9	POS. OR TENT ID	CONC. (%HEB)
1	10.36	10-OXO-UNDECANOIC ACID	676006	1		T	480.00
2	9.36	4-METHYLHEXANAL	41065978	1		T	250.00
3	9.36	%HEPTANOIC ACID	111148	1		P	200.00
4	9.36	3,6-DIMETHYLOCTANOIC ACID	4812297	1		T	100.00
5	9.36	3,4-DIMETHYLBENZOIC ACID	619045	1		P	197.00
6	9.36	CIS-1,3-DICHLOROCYCLOHEXANE	24955633		1	T	115.00
7	8.36	3-HEXANOL	623370	1		T	53.00
8	8.36	2-PYRROLIDONE	616455	1		P	50.00
9	8.36	6-UNDECANOL	23708567	1		T	35.00
10	8.36	[illegible]2-OCTANEDIOL	1117868	1		T	40.00
11	8.36	[illegible]-2-ETHYL-3-METHYL-2-BUTENEDIOIC ACID	41654095	1		T	96.00
12	8.36	[illegible]ETYL-P-TOLUIC ACID	15482549	1		T	38.00
13	8.36	%NO[illegible]NEDIOIC ACID	123999	1		P	70.00
14	8.36	9-OXODECANOIC ACID	1422260	1		T	75.00
15	8.36	1,3-DIMETHYL-2-(2-ISOPROPYLPHENYL)ETHYLCYCLOHEXANE CARBOXILIC ACID	6080	1		T	45.00
16	8.36	1,2,3,4,4A,9,10,10A-OCTAHYDRO-1,4A-DIMETHYL-7-(1-METHYLETHYL)-1-PHENANTHRENEC	5155704	1		T	74.00
17	7.36	4-HEPTANONE	123193	1		T	18.00
18	7.36	2-METHYL BENZOIC ACID	118901	1		P	10.00
19	7.36	%UNDECANOIC ACID	112378	1		P	16.00
20	7.36	10-UNDECENOIC ACID	112389	1		T	19.00
21	7.36	0-BROMOPHENOL	95567	1		T	10.00
22	7.36	CIS-2,3-DIMETHYLBUTENEDIOIC ACID	488211	1		P	35.00
23	7.36	TRIDECANOIC ACID	638539	1		P	15.00
24	7.36	3-HYDROXYNONANOIC ACID	33796871	1		T	22.00
25	7.36	OCTANEDIOIC ACID	505486	1		P	16.00
26	7.36	5-HEXYLDIHYDROFURANONE	706149	1		T	18.00
27	7.36	1,4-BENZOTHIAZIN-3-ONE	5325202	1		T	8.00
28	7.36	N-PHENYL ACETAMIDE	103844	1		T	10.00
29	7.36	8,11,14-OCTADECATRIENOIC ACID	4906916	1		T	9.00
30	7.36	OCTAHYDRO-1,4A-DIMETHYL-1-PHENANTHRENE CARBOXILIC ACID, METHYL ESTER	3650042	1		T	17.00
31	7.36	1,1-DICHLOROCYCLOHEXANE	2108921		1	T	10.00
32	7.36	%DIBROMOCHLOROMETHANE	124481		1	P	27.00
33	7.36	%TRIBROMOMETHANE	75252		1	P	14.00
34	7.36	CIS-1-BROMO-2-CHLOROCYCLOHEXANE	51422754		1	T	24.00
35	7.36	0-NITROTOLUENE	88722		1	T	15.00
36	7.36	2,6-DINITROTOLUENE	606202		1	P	10.00
37	7.36	%1-METHYL-2,4-DINITROBENZENE	121142		1	P	23.00
38	7.36	%BROMODICHLOROMETHANE	75274		1	P	10.00
39	7.36	4,8,12-TRIMETHYL-3,7,11-TRIDECATRIENITRILE	6006015		1	T	18.00
40	6.36	BROMOMETHANE	74839	1		T	3.00
41	6.36	%DICHLOROACETIC ACID	79436	1		P	5.00
42	6.36	4-METHYL-4-NITROPENTANOIC ACID	23102025	1		T	10.00
43	6.36	3-METHYLBENZOIC ACID	99047	1		P	8.00
44	6.36	4-METHYLBENZOIC ACID	99945	1		P	5.00
45	6.36	%BENZENE ACETIC ACID	103822	1		P	6.00

(continued)

TABLE B3. (continued)

COMPOUNDS FOUND IN CONCENTRATE BY RELATIVE SIZE (PART I)
UNDER FRACTION, 1=FOUND ON GC COLUMN 1, 2=FOUND ON GC COLUMN 2, 3=FOUND ON BOTH GC COLUMN 1 AND GC COLUMN 2
CINCINNATI IV GAC FEED CA PERMEATE

Code Name T4R3

SEQ NO.	RS	SYSTEMATIC NAME	CAS NO.	FRACTION 2	FRACTION 9	POS. OR TENT ID	CONC. (%HEB)
46	6.36	2,4-DIMETHYL BENZOIC ACID	611018	1		P	13.00
47	6.36	%3-PHENYLPROPIONIC ACID	501520	1		P	4.00
48	6.36	2-(1-METHYLETHYL)BENZOIC ACID	2438042	1		T	5.00
49	6.36	3,5-DIMETHYL BENZOIC ACID	499069	1		P	7.00
50	6.36	ANTEISOTRIDECANOIC ACID	26403145	1		T	9.00
51	6.36	ACETIC ACID, 2-METHYL PHENYL ESTER	533186	1		T	6.00
52	6.36	%*+$2,4-DICHLOROPHENOL	120832	1		P	11.00
53	6.36	5-DODECANOL	10203335	1		T	8.00
54	6.36	2,5-DICHLOROPHENOL	583788	1		P	2.00
55	6.36	ISO-TRIDECANOIC ACID	25448242	1		T	5.00
56	6.36	1,4-DICHLORO-2,5-DIHYDROXY BENZENE	824691	1		T	4.00
57	6.36	4-METHOXYBENZOIC ACID	100094	1		P	5.00
58	6.36	2-(4-CHLOROPHENOXY)-2-METHYLPROPANOIC ACID	882097	1		P	5.00
59	6.36	%+$1,2-DICHLORO BENZENE	95501		1	P	9.00
60	6.36	BENZONITRILE	100470		1	P	5.00
61	6.36	TRIMETHYLNAPHTHALENE	317		1	T	4.00
62	6.36	%BENZENEACETONITRILE	140294		1	P	6.00
63	6.36	1,1,1,5,5,5-HEXACHLOROPENTANE	30353594		1	T	4.00
64	6.36	P-CHLORO-2-NITHROANILINE	89634		1	T	4.00
65	6.36	%+NAPHTHALENE	91203		1	P	9.00
66	6.36	3-CHLOROCYCLOHEXENE	2441976		1	T	5.00
67	5.36	%$(1-METHYL ETHYL) BENZENE	98828		1	P	1.00
68	5.36	%+$1,3-DICHLOROBENZENE	541731		1	P	1.50
69	5.36	%+$1,1≠-OXYBIS[2-CHLOROETHANE]	111444		1	P	1.00
70	5.36	5-(PENTYLOXY)-2-PENTENE	56052858		1	T	1.50
71	5.36	%2-OCTANONE	111137		1	T	1.00
72	5.36	4-METHYLBENZALDEHYDE OXIME	3717155		1	T	1.00
73	5.36	BENZOIC ACID, BUTYL ESTER	136607		1	P	1.00
74	5.36	P-NITROTOLUENE	99990		1	T	3.00
75	5.36	%2-ETHYL NAPHTHALENE	939275		1	P	1.00
76	5.36	1,8-DIMETHYLNAPHTHALENE	569415		1	T	3.00
77	5.36	%1,1≠-OXYBISBENZENE	101848		1	P	1.00
78	5.36	(1-METHYLETHYL)NAPHTHALENE	29253369		1	T	1.00
79	5.36	3-METHYLBIPHENYL	643936		1	T	3.00
80	5.36	4-METHYL BIPHENYL	644386		1	T	2.00
81	5.36	TRIMETHYLNAPHTHALENE	316		1	P	0.50
82	5.36	3,3-DIMETHYLBENZENE	612759		1	T	1.00
83	5.36	4,4-DIMETHYLBIPHENYL	613332		1	T	1.00
84	5.36	[1,1≠-BICYCLOPENTYL]-2-ONE	4884246		1	T	2.50
85	5.36	%*+$NITROBENZENE	98953		1	P	2.00
86	5.36	1-ISOCYANONAPHTHALENE	1984049		1	T	2.00
87	5.36	BROMODIMETHYLNAPHTHALENE	5334792		1	T	3.00
88	5.36	1-METHYL-9H-FLUORENE	1730376		1	P	1.00
89	5.36	3,5-BIS(1,1-DIMETHYLETHYL)-4-HYDROXY-2,4-CYCLOHEXADIEN-1-ONE	54965434		1	T	1.00
90	4.36	2,3,6-TRIMETHYLNAPHTHALENE	829265		1	P	1.00

TABLE B4. COMPOUND IDENTIFICATION RESULTS FOR THE CINCINNATI GAC CONTACTOR A SAMPLE, T4R1, PRE-GAC 10-FOLD CELLULOSE ACETATE RO BRINE

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COMPOUNDS FOUND IN CONCENTRATE BY RELATIVE SIZE (PART I)
UNDER FRACTION, 1=FOUND ON GC COLUMN 1, 2=FOUND ON GC COLUMN 2, 3=FOUND ON BOTH GC COLUMN 1 AND GC COLUMN 2
CINCINNATI IV GAC FEED 10 X CA RO

Code Name T4R1

SEQ NO.	RS	SYSTEMATIC NAME	CAS NO.	FRACTION 2	FRACTION 9	POS. OR TENT ID	CONC. (%HEB)
1	8.36	%HEPTANOIC ACID	111148	1		T	84.00
2	8.36	%BENZOIC ACID	65850	1		P	70.00
3	8.36	CIS-2,3-DIMETHYLBUTENEDIOIC ACID	488211	1		P	57.00
4	8.36	CIS-2-ETHYL-3-METHYL-2-BUTENEDIOIC ACID	41654095	1		T	137.00
5	8.36	10-OXO-UNDECANOIC ACID	676006	1		T	134.00
6	8.36	1,3-DIMETHYL-2-(2-ISOPROPYLPHENYL)ETHYLCYCLOHEXANE CARBOXILIC ACID	6080	1		T	84.00
7	7.36	3,6-DIMETHYLOCTANOIC ACID	4812297	1		T	33.00
8	7.36	2-DODECENAL	4826624	1		T	26.00
9	7.36	10-UNDECENOIC ACID	112389	1		T	14.00
10	7.36	4-OXO-NONANOIC ACID	6064524	1		T	28.00
11	7.36	3-HYDROXYNONANOIC ACID	33796871	1		T	34.00
12	7.36	ISOPENTADECANOIC ACID	544	1		T	20.00
13	7.36	2-(4-CHLOROPHENOXY)-2-METHYLPROPANOIC ACID	882097	1		P	22.00
14	7.36	9-OXODECANOIC ACID	1422260	1		T	35.00
15	7.36	HEPTADECENOIC ACID	26265996	1		T	40.00
16	7.36	%*(2,4-DICHLOROPHENOXY)ACETIC ACID	94757	1		T	15.00
17	7.36	1,1,1,5,5,5-HEXACHLOROPENTANE	30353594		1	T	11.00
18	6.36	2-METHYL BENZOIC ACID	118901	1		P	80.00
19	5.36	1,1≠-(3,3-DIMETHYL-1-BUTENYLIDENE)BISBENZENE	23586643		1	T	0.50
20	5.36	%*NAPHTHALENE	91203		1	P	22.00
21	4.36	4-PHENYLBICYCLOHEXYL	20273272		1	T	0.50
22	4.36	%1-METHYL-2,4-DINITROBENZENE	121142		1	P	1.00
23	4.36	%9H-FLUOREN-9-ONE	486259		1	P	0.50
24	4.36	%DIBROMOCHLOROMETHANE	124481		1	P	1.00
25	4.36	%TRIBROMOMETHANE	75252		1	P	0.50
26	4.36	1,2-DICHLOROCYCLOHEXANE	822866		1	T	1.00
27	4.36	%1-PHENYLETHANONE	98862		1	P	1.00
28	4.36	O-NITROTOLUENE	88722		1	T	0.50
29	4.36	%BENZENEACETONITRILE	140294		1	P	1.00
30	4.36	%*2-CHLORO-BENZENEAMINE	95512		1	P	1.00

TABLE B5. COMPOUND IDENTIFICATION RESULTS FOR THE CINCINNATI GAC CONTACTOR A SAMPLE, T4R2, PRE-GAC 100-FOLD CELLULOSE ACETATE RO BRINE

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COMPOUNDS FOUND IN CONCENTRATE BY RELATIVE SIZE (PART I)

UNDER FRACTION, 1=FOUND ON GC COLUMN 1, 2=FOUND ON GC COLUMN 2, 3=FOUND ON BOTH GC COLUMN 1 AND GC COLUMN 2

CINCINNATI IV GAC FEED 100 X CA RO

Code Name T4R2

SEQ NO.	RS	SYSTEMATIC NAME	CAS NO.	FRACTION 2	FRACTION 9	POS. OR TENT ID	CONC. (%HEB)
1	9.36	%BENZOIC ACID	65850	1		P	32.00
2	8.36	%HEXANOIC ACID	142621	1		P	29.00
3	8.36	2-ETHYLHEXANOIC ACID	149575	1		P	59.00
4	8.36	%HEPTANOIC ACID	111148	1		P	46.00
5	8.36	CIS-2,3-DIMETHYLBUTENEDIOIC ACID	488211	1		P	44.00
6	8.36	CIS-2-ETHYL-3-METHYL-2-BUTENEDIOIC ACID	41654095	1		T	65.00
7	8.36	2-ACETYL-P-TOLUIC ACID	15482549	1		T	27.00
8	8.36	3-HYDROXYNONANOIC ACID	33796871	1		T	14.00
9	8.36	2-(4-CHLOROPHENOXY)-2-METHYLPROPANOIC ACID	882097	1		P	12.00
10	8.36	%NONANEDIOIC ACID	123999	1		P	15.00
11	8.36	5-HEXYLDIHYDROFURANONE	706149	1		T	15.00
12	8.36	9-OXODECANOIC ACID	1422260	1		T	26.00
13	8.36	10-OXO-UNDECANOIC ACID	676006	1		T	44.00
14	8.36	1,3-DIMETHYL-2-(2-ISOPROPYLPHENYL)ETHYLCYCLOHEXANE CARBOXILIC ACID	6080	1		T	15.00
15	8.36	1,2,3,4,4A,9,10,10A-OCTAHYDRO-1,4A-DIMETHYL-7-(1-METHYLETHYL)-1-PHENANTHRENEC	5155704	1		T	100.00
16	8.36	2-NONENAL	2463538	1		T	16.00
17	8.36	1.-UNDECENOIC ACID	112389	1		T	19.00
18	7.36	DIVINYL MERCURY	1119206	1		T	2.00
19	7.36	2-METHYL BENZOIC ACID	118901	1		P	6.00
20	7.36	ACETIC ACID, 2-METHYL PHENYL ESTER	533186	1		T	5.00
21	7.36	ISOPALMITIC ACID	545	1		P	4.00
22	7.36	%3,6-DICHLORO-2-METHOXYBENZOIC ACID	1918009	1		T	3.00
23	7.36	1-(3,4-DIHYDROXYPHENYL)ETHANONE	1197097	1		T	9.00
24	7.36	OCTAHYDRO-1,4A-DIMETHYL-1-PHENANTHRENE CARBOXILIC ACID, METHYL ESTER	3650042	1		T	11.00
25	7.36	12-METHYLTETRADECANOIC ACID	5502943	1		T	9.00
26	7.36	3-HYDROXYCAPRIC ACID	14292263	1		P	4.00
27	7.36	ANTEISOHEPTADECANOIC ACID	457	1		P	7.00
28	7.36	%1,2-BENZENEDICARBOXYLIC ACID	88993	1		P	5.00
29	6.36	1,1,1,5,5,5-HEXACHLOROPENTANE	30353594		1	T	6.00
30	6.36	%+NAPHTHALENE	91203		1	P	6.00
31	4.36	3-HEPTANOL	589822		1	T	0.50
32	4.36	(1-METHYLUNDECYL)BENZENE	2719611		1	T	1.00
33	4.36	%+ANTHRACENE	120127		1	P	1.00
34	4.36	DICHLOROBUTENE	110576		1	T	0.50

TABLE B6. COMPOUND IDENTIFICATION RESULTS FOR THE CINCINNATI GAC CONTACTOR A SAMPLE, T4R6, PRE-GAC, 200-FOLD CELLULOSE ACETATE RO BRINE

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COMPOUNDS FOUND IN CONCENTRATE BY RELATIVE SIZE (PART I)
UNDER FRACTION, 1=FOUND ON GC COLUMN 1, 2=FOUND ON GC COLUMN 2, 3=FOUND ON BOTH GC COLUMN 1 AND GC COLUMN 2
CINCINNATI IV GAC FEED 200 X CA RO

Code Name R4R6

SEQ NO.	RS	SYSTEMATIC NAME	CAS NO.	FRACTION 2	FRACTION 4	POS. OR TENT ID	CONC. (%HEB)
1	9.36	CIS-2-ETHYL-3-METHYL-2-BUTENEDIOIC ACID	41654095	1		P	100.00
2	8.36	%BENZALDEHYDE	100527		1	P	30.00
3	8.36	1,3,5-TRIMETHYL-1,3,5-TRIAZINE-2,4,6-TRIONE	827167		1	P	116.00
4	7.36	3,6-DIMETHYLOCTANOIC ACID	4812297	1		T	15.00
5	7.36	3-HYDROXYNONANOIC ACID	33796871	1		T	16.00
6	7.36	2-(4-CHLOROPHENOXY)-2-METHYLPROPANOIC ACID	882097	1		P	29.00
7	7.36	%NONANEDIOIC ACID	123999	1		P	13.00
8	7.36	9-OXODECANOIC ACID	1422260	1		T	12.00
9	7.36	%3,6-DICHLORO-2-METHOXYBENZOIC ACID	1918009	1		T	6.00
10	7.36	10-OXO-UNDECANOIC ACID	676006	1		T	5.00
11	7.36	%DIBROMOCHLOROMETHANE	124481		1	P	7.00
12	7.36	DIMETHYL-(1-METHYLETHYL)BENZENE	103		1	T	8.00
13	7.36	2,5-HEXANEDIONE	110134		1	P	9.00
14	7.36	%PHOSPHORIC ACID, TRIETHYLESTER	78400		1	P	7.00
15	7.36	%1-METHYL-2-PYRROLIDINONE	872504		1	P	8.00
16	7.36	METHOXYPROPOXY PROPOXY PROPANOL	400		1	P	8.00
17	7.36	METHOXYPROPOXY PROPOXY PROPANOL	401		1	P	7.00
18	7.36	METHOXYPROPOXY PROPOXY PROPANOL	402		1	P	10.00
19	7.36	METHOXYPROPOXY PROPOXY PROPANOL	403		1	P	7.00
20	7.36	%BENZENEMETHANOL	100516		1	T	10.00
21	7.36	5,6,7,7A-TETRAHYDRO-4,4,7A-TRIMETHYL-2(4H)-BENZOFURANONE	17092921		1	T	10.00
22	7.36	4,7,10-TRIMETHYL-2,5,8,11-TETRAOXATETRADECAN-13-OL	20324349		1	T	16.00
23	7.36	%7-OXABICYCLO[4.1.0]HEPTANE	286204		1	T	29.00
24	7.36	CYCLIC TETRAMETHYLENE ADIPATE	777357		1	T	19.00
25	6.36	%BENZENE ACETIC ACID	103822	1		P	6.00
26	6.36	1-(2-METHOXYPROPOXY)-2-PROPANOL	13429077	1		T	10.00
27	6.36	%2-HYDROXYBENZOIC ACID	69727	1		P	11.00
28	6.36	CIS-2,3-DIMETHYLBUTENEDIOIC ACID	488211	1		P	10.00
29	6.36	ACETIC ACID, 2-METHYL PHENYL ESTER	533186	1		T	10.00
30	6.36	5-HEPTYL DIHYDRO-2-FURANONE	104676	1		T	8.00
31	6.36	OCTAHYDRO-1,4A-DIMETHYL-1-PHENANTHRENE CARBOXILIC ACID, METHYL ESTER	3650042	1		T	10.00
32	6.36	4-(1-METHYLETHYL)BENZOIC ACID	536663	1		T	8.00
33	6.36	PROPYLENE GLYCOL MONOBUTYL ETHER	5086		1	T	5.00
34	6.36	N,N-DIETHYFORMAMIDE	617845		1	P	6.00
35	6.36	1-HEPTANOL	111706		1	T	5.00
36	6.36	%1,7,7-TRIMETHYLBICYCLO[2.2.1]HEPTAN-2-ONE	76222		1	P	5.00
37	6.36	3-METHYL-2-CYCLOPENTEN-1-ONE	2758181		1	P	3.00
38	6.36	5,5-DIMETHYL-2(5H)-FURANONE	20019641		1	T	6.00
39	6.36	%1-PHENYLETHANONE	98862		1	P	3.50
40	6.36	%TRIBUTYL PHOSPHATE	126738		1	P	3.00
41	6.36	2,2'-OXYBIS[2-METHYLPROPANE]	6163662		1	T	9.00
42	6.36	4-HYDROXY-4-METHYLCYCLOHEXANONE	17429026		1	T	9.00
43	6.36	2,2,6-TRIMETHYL-1,4-CYCLOHEXANEDIONE	20547393		1	T	7.00
44	5.36	DIMETHYL-(1-METHYLETHYL)BENZENE	104		1	T	1.50
45	5.36	1,1,2-TRICHLORO-1-PROPENE	21400259		1	T	2.00
46	5.36	2,6-BIS(1,1-DIMETHYL ETHYL)-4-ETHYL PHENOL	4130421		1	T	3.00

TABLE B7. COMPOUND IDENTIFICATION RESULTS FOR THE CINCINNATI GAC CONTACTOR A SAMPLE, T4E1, PRE-GAC 10 LITERS, NO RO PROCESSING

COMPOUNDS FOUND IN CONCENTRATE BY RELATIVE SIZE (PART I)
UNDER FRACTION, 1=FOUND ON GC COLUMN 1, 2=FOUND ON GC COLUMN 2, 3=FOUND ON BOTH GC COLUMN 1 AND GC COLUMN 2
CINCINNATI 4 GAC FEED

Code Name T4E1

SEQ NO.	RS	SYSTEMATIC NAME	CAS NO.	FRACTION		POS. OR TENT ID	CONC. (%HEB)
				2	9		
1	8.36	CIS-2,3-DIMETHYLBUTENEDIOIC ACID	488211	1		P	40.00
2	8.36	CIS-2-ETHYL-3-METHYL-2-BUTENEDIOIC ACID	41654095	1		T	68.00
3	7.36	%DICHLOROACETIC ACID	79436	1		P	15.00
4	7.36	2,2-DICHLOROETHANOL	598389	1		T	24.00
5	7.36	ISOPENTADECANOIC ACID	544	1		P	14.00
6	7.36	4-METHOXYBENZOIC ACID	100094	1		P	5.00
7	7.36	2-(4-CHLOROPHENOXY)-2-METHYLPROPANOIC ACID	882097	1		P	11.00
8	7.36	HEPTADECENOIC ACID	26265996	1		T	16.00
9	7.36	8,11-OCTADECADIENOIC ACID	2197526	1		T	28.00
10	7.36	2,2≠-BI-1,3-DIOXOLANE	6705891	1		T	19.00
11	7.36	%DIBROMOCHLOROMETHANE	124481		1	P	27.00
12	7.36	%*+$1,4-DICHLOROBENZENE	106467		1	P	3.00
13	7.36	%TRIBROMOMETHANE	75252		1	P	12.00
14	7.36	1,1,1.5,5,5-HEXACHLOROPENTANE	30353594		1	T	15.00
15	6.36	%BENZENE ACETIC ACID	103822	1		P	4.00
16	6.36	%3-PHENYLPROPIONIC ACID	501520	1		P	4.00
17	6.36	TRIDECANOIC ACID	638539	1		P	4.00
18	6.36	ISOMYRISTIC ACID	543	1		P	4.00
19	6.36	2-PHENYL BUTANOIC ACID	90277	1		T	2.00
20	6.36	ANTEISOHEPTADECANOIC ACID	457	1		P	6.00
21	6.36	%*(2,4-DICHLOROPHENOXY)ACETIC ACID	94757	1		T	6.00
22	6.36	%BROMODICHLOROMETHANE	75274		1	P	3.00
23	6.36	%+$1,2-DICHLORO BENZENE	95501		1	P	5.00
24	6.36	%1-PHENYL-1-PROPANONE	93550		1	P	5.00
25	6.36	O-NITROTOLUENE	88722		1	T	8.00
26	6.36	%BENZENEACETONITRILE	140294		1	P	4.00
27	6.36	2,6-DINITROTOLUENE	606202		1	P	5.00
28	6.36	%1-METHYL-2,4-DINITROBENZENE	121142		1	P	9.00
29	5.96	%*2-CHLORO-BENZENEAMINE	95512	1		P	3.00
30	5.36	4-OXO-PENTANOIC ACID	123762	1		P	6.00
31	5.36	%2-HYDROXYBENZOIC ACID	69727	1		P	3.00
32	5.36	ACETIC ACID, 2-METHYL PHENYL ESTER	533186	1		T	3.00
33	5.36	%+$1,3-DICHLOROBENZENE	541731		1	P	1.00
34	5.36	%+$1,1≠-OXYBIS(2-CHLOROETHANE)	111444		1	P	1.00
35	5.36	BENZONITRILE	100470		1	P	3.00
36	5.36	P-NITROTOLUENE	99990		1	T	1.50
37	4.36	(DICHLOROMETHYL)NAPHTHALENE	17180266		1	T	1.00
38	4.36	%BROMOCYCLOHEXANE	108850		1	T	1.00
39	4.36	1,1,2,3-TETRACHLOROPROPANE	18495302		1	T	1.00
40	4.36	2,4-DICHLORO-1-NITROBENZENE	611063		1	T	0.50
41	4.36	%1,1≠-OXYBISBENZENE	101848		1	P	0.50
42	4.36	2,3-DIHYDRO-1,1,3-TRIMETHYL-3-PHENYL-1H-INDENE	3910358		1	T	0.50

TABLE B8. COMPOUND IDENTIFICATION RESULTS FOR THE CINCINNATI GAC CONTACTOR A SAMPLE, T4G1, POST-GAC, 10 LITERS, NO RO PROCESSING

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COMPOUNDS FOUND IN CONCENTRATE BY RELATIVE SIZE (PART I)
UNDER FRACTION, 1=FOUND ON GC COLUMN 1, 2=FOUND ON GC COLUMN 2, 3=FOUND ON BOTH GC COLUMN 1 AND GC COLUMN 2
CINCINNATI IV POST GAC
Code Name T4G1

SEQ NO.	RS	SYSTEMATIC NAME	CAS NO.	FRACTION 2	FRACTION 9	POS. OR TENT ID	CONC. (%HEB)
1	9.36	%BENZOIC ACID	65850	1		P	16.00
2	8.36	CIS-2,3-DIMETHYLBUTENEDIOIC ACID	488211	1		P	88.00
3	8.36	CIS-2-ETHYL-3-METHYL-2-BUTENEDIOIC ACID	41654095	1		T	96.00
4	8.36	CIS-9-HEXADECENOIC ACID	2091294	1		T	80.00
5	7.36	%1-HEXADECANOL	36653824	1		P	26.00
6	7.36	4-(1,5-DIMETHYL-3-OXOHEXYL)CYCLOHEXANECARBOXYLIC ACID	38963916	1		T	13.00
7	6.36	4-HEPTANONE	123193	1		T	9.00
8	6.36	4-OXO-NONANOIC ACID	6064524	1		T	4.00
9	6.36	1,1,1,5,5,5-HEXACHLOROPENTANE	30353594		1	T	4.00
10	5.36	%HEPTANOIC ACID	111148	1		P	4.00
11	5.36	TRIDECANOIC ACID	638539	1		P	4.00
12	5.36	ISOMYRISTIC ACID	543	1		P	4.00
13	5.36	%1-DODECANOL	112538	1		P	2.00
14	5.36	%+NAPHTHALENE	91203		1	P	2.50

TABLE B9. COMPOUND IDENTIFICATION RESULTS FOR THE CINCINNATI GAC CONTACTOR A SAMPLE, T4G2, POST-GAC, 200-FOLD CELLULOSE ACETATE RO BRINE

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COMPOUNDS FOUND IN CONCENTRATE BY RELATIVE SIZE (PART I)
UNDER FRACTION, 1=FOUND ON GC COLUMN 1, 2=FOUND ON GC COLUMN 2, 3=FOUND ON BOTH GC COLUMN 1 AND GC COLUMN 2
CINCINNATI 4 POST GAC 200 X CA RO 10 LITERS

Code Name T4G2

SEQ NO.	RS	SYSTEMATIC NAME	CAS NO.	FRACTION 2	FRACTION 4	POS. OR TENT ID	CONC. (%HEB)
1	21.36	1,3-DIMETHYL-2-(2-ISOPROPYLPHENYL)ETHYLCYCLOHEXANE CARBOXILIC ACID	6080	1		T	17.00
2	9.36	3,4-DICHLOROBENZOIC ACID	51445	1		P	107.00
3	8.36	2-METHOXYETHANOL	109864	1		T	35.00
4	8.36	CIS-2,3-DIMETHYLBUTENEDIOIC ACID	488211	1		P	98.00
5	8.36	CIS-2-ETHYL-3-METHYL-2-BUTENEDIOIC ACID	41654095	1		T	67.00
6	7.36	3,6-DIMETHYLOCTANOIC ACID	4812297	1		T	23.00
7	7.36	DIETHYLENE GLYCOL	111466	1		T	20.00
8	7.36	OCTAHYDRO-1,4A-DIMETHYL-1-PHENANTHRENE CARBOXILIC ACID, METHYL ESTER	3650042	1		T	22.00

TABLE B10. COMPOUND IDENTIFICATION RESULTS FOR THE CINCINNATI GAC CONTACTOR A SAMPLE, T4Y2, PRE-GAC 10-LITER XAD-2 CONCENTRATE: SULFITE PRESERVED

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COMPOUNDS FOUND IN CONCENTRATE BY RELATIVE SIZE (PART I)
UNDER FRACTION, 1=FOUND ON GC COLUMN 1, 2=FOUND ON GC COLUMN 2, 3=FOUND ON BOTH GC COLUMN 1 AND GC COLUMN 2
CINCINNATI IV GAC FEED, XAD ETHER ELUATE, WITH SULFITE

Code Name T4Y2

SEQ NO.	RS	SYSTEMATIC NAME†	CAS NO.	FRACTION 2	FRACTION 9	POS. OR TENT ID	CONC. (%HEB)
1	9.36	%BENZOIC ACID	65850	1		P	200.00
2	9.36	%BENZOIC ACID METHYL ESTER	93583		1	P	233.00
3	8.36	%DODECANOIC ACID	143077	1		P	74.00
4	8.36	CIS-2-ETHYL-3-METHYL-2-BUTENEDIOIC ACID	41654095	1		T	96.00
5	8.36	%+$1,2-DICHLORO BENZENE	95501		1	P	60.00
6	7.96	†%$1,3-DIMETHYLBENZENE	108383	1		P	22.00
7	7.60	† $ETHYLBENZENE	100414	1		P	8.00
8	7.36	2-ETHYLHEXANOIC ACID	149575	1		P	28.00
9	7.36	%DICHLOROACETIC ACID	79436	1		P	16.00
10	7.36	%OCTANOIC ACID	124072	1		P	14.00
11	7.36	%NONANOIC ACID	112050	1		P	25.00
12	7.36	%DECANOIC ACID	334485	1		P	19.00
13	7.36	%BENZENE ACETIC ACID	103822	1		P	13.00
14	7.36	CIS-2,3-DIMETHYLBUTENEDIOIC ACID	488211	1		P	22.00
15	7.36	P-ETHYLBENZOIC ACID	619647	1		P	13.00
16	7.36	%TETRADECANOIC ACID	544638	1		P	32.00
17	7.36	PHENOXY ACETIC ACID	122598	1		P	11.00
18	7.36	%NONANEDIOIC ACID	123999	1		P	30.00
19	7.36	%DIBROMOCHLOROMETHANE	124481		1	P	14.00
20	7.36	ETHYLBENZALDEHYDE (ISOMER UNKNOWN)	53951501		1	T	13.00
21	7.36	%+NAPHTHALENE	91203		1	P	11.00
22	6.36	%1-PROPANOL	71238	1		T	7.00
23	6.36	%PENTANOIC ACID	109524	1		P	7.00
24	6.36	1-CHLORO-2-PROPANOL	127004	1		T	9.00
25	6.36	2,2≠-BI-1,3-DIOXOLANE	6705891	1		T	9.00
26	6.36	2,3,3-TRICHLORO-2-PROPENOIC ACID	2257354	1		T	6.00
27	6.36	3-METHYLBENZOIC ACID	99047	1		P	3.00
28	6.36	ALPHA-METHYLBENZENEACETIC ACID	492375	1		P	4.00
29	6.36	%2-HYDROXYBENZOIC ACID	69727	1		P	6.00
30	6.36	O-ETHYLBENZOIC ACID	28134318	1		T	10.00
31	6.36	TETRACHLOROBUTENOIC ACID	5085	1		T	6.00
32	6.36	%3-PHENYLPROPIONIC ACID	501520	1		P	7.00
33	6.36	3,5-DIMETHYL BENZOIC ACID	499069	1		P	7.00
34	6.36	2-ACETYL-P-TOLUIC ACID	15482549	1		T	5.00
35	6.36	%*+PHENOL	108952	1		P	6.00
36	6.36	OCTANEDIOIC ACID	505486	1		P	6.00
37	6.36	4-(1,5-DIMETHYL-3-OXOHEXYL)-1-CYCLOHEXENE-1-CARBOXYLIC ACID	17844074	1		T	8.00
38	6.36	(2,5-DIMETHYLBENZENE)BUTANOIC ACID	1453061	1		T	7.00
39	6.36	4-METHOXYBENZOIC ACID	100094	1		P	8.00
40	6.36	2-(4-CHLOROPHENOXY)-2-METHYLPROPANOIC ACID	882097	1		P	9.00
41	6.36	2-HYDROXY-1H-ISOINDOLE-1,3(2H)-DIONE	524389	1		T	6.00
42	6.36	%1,2-BENZENEDICARBOXYLIC ACID	88993	1		P	8.00
43	6.36	%*(2,4-DICHLOROPHENOXY)ACETIC ACID	94757	1		T	5.00
44	6.36	%$1,4-DIMETHYBENZENE	106423		1	P	8.00
45	6.36	%$1,2-DIMETHYLBENZENE	95476		1	P	10.00

(continued)

TABLE B10. (continued)

COMPOUNDS FOUND IN CONCENTRATE BY RELATIVE SIZE (PART I)
UNDER FRACTION, 1=FOUND ON GC COLUMN 1, 2=FOUND ON GC COLUMN 2, 3=FOUND ON BOTH GC COLUMN 1 AND GC COLUMN 2
CINCINNATI IV GAC FEED, XAD ETHER ELUATE, WITH SULFITE

Code Name T4Y2

SEQ NO.	RS	SYSTEMATIC NAME†	CAS NO.	FRACTION		POS. OR TENT ID	CONC. (XMEB)
				2	9		
46	6.36	† 1,2,4-TRIMETHYL BENZENE	95636		1	P	9.00
47	6.36	%TRIBROMOMETHANE	75252		1	P	8.00
48	6.36	0-NITROTOLUENE	88722		1	T	7.00
49	6.36	† METHYLP-ETHYLBENZOATE	7364207		1	P	5.00
50	6.36	%1-METHYL-2,4-DINITROBENZENE	121142		1	P	8.00
51	6.36	%BENZALDEHYDE	100527		1	P	6.00
52	5.36	† 1-ETHYL-3-METHYL BENZENE	620144		1	P	3.00
53	5.36	† %1,3,5-TRIMETHYL BENZENE	108678		1	P	2.00
54	5.36	BENZONITRILE	100470		1	P	2.00
55	5.36	† %BENZOIC ACID, ETHYL ESTER	93890		1	P	3.00
56	5.36	HEXADECANOIC ACID, METHYL ESTER	112390		1	P	1.00
57	5.36	HEXADECANOIC ACID, ETHYL ESTER	628977		1	P	2.00
58	5.36	2,6-DINITROTOLUENE	606202		1	P	3.00
59	5.36	† 1-METHYL-4-PROPYLBENZENE	1074551		1	P	2.00
60	5.36	† 1-ETHYL-3,5-DIMETHYL BENZENE	934747		1	P	3.00
61	5.36	† 1,2,3-TRIMETHYL BENZENE	526738		1	P	3.00
62	5.36	† 1-METHYL-2-PROPYL BENZENE	1074175		1	P	1.00
63	5.36	† DIMETHYL ETHYL BENZENE	208		1	T	2.00
64	5.36	† DIMETHYL ETHYL BENZENE	201		1	T	2.00
65	5.36	† 4-ETHYL-1,2-DIMETHYL BENZENE	934805		1	P	4.00
66	4.36	ETHYL DICHLOROACETATE	535159		1	T	1.00

† A PROBABLE OR POSSIBLE XAD-2 RESIN BLEED ARTIFACT.

TABLE B11. COMPOUND IDENTIFICATION RESULTS FOR THE CINCINNATI GAC CONTACTOR A SAMPLE, T4Y4, PRE-GAC 10-LITER XAD-2 CONCENTRATE

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COMPOUNDS FOUND IN CONCENTRATE BY RELATIVE SIZE (PART I)
UNDER FRACTION, 1=FOUND ON GC COLUMN 1, 2=FOUND ON GC COLUMN 2, 3=FOUND ON BOTH GC COLUMN 1 AND GC COLUMN 2
CINCINNATI IV GAC FEED, XAD ETHER ELUATE, WITHOUT SULFITE

Code Name T4Y4

SEQ NO.	RS	SYSTEMATIC NAME†	CAS NO.	FRACTION 2	FRACTION 3	POS. OR TENT ID	CONC. (%HEB)
1	9.36	+ %BENZOIC ACID METHYL ESTER	93583		1	P	124.00
2	8.36	%NONANOIC ACID	112050	1		P	31.00
3	8.36	%DODECANOIC ACID	143077	1		P	83.00
4	8.36	O-ETHYLBENZOIC ACID	28134318	1		T	39.00
5	8.36	CIS-2-ETHYL-3-METHYL-2-BUTENEDIOIC ACID	41654095	1		T	39.00
6	8.36	%TETRADECANOIC ACID	544638	1		P	40.00
7	8.36	%NONANEDIOIC ACID	123999	1		P	50.00
8	8.36	%+$1,2-DICHLORO BENZENE	95501		1	P	52.00
9	7.36	%1,4-DIOXANE	123911	1		T	39.00
10	7.36	2-METHOXY-1-PROPANOL	1589475	1		T	13.00
11	7.36	2-ETHYLHEXANOIC ACID	149575	1		P	13.00
12	7.36	%HEPTANOIC ACID	111148	1		P	10.00
13	7.36	%DICHLOROACETIC ACID	79436	1		P	17.00
14	7.36	%OCTANOIC ACID	124072	1		P	17.00
15	7.36	P-ETHYLBENZOIC ACID	619647	1		P	12.00
16	7.36	ISOMYRISTIC ACID	543	1		P	11.00
17	7.36	%DECANOIC ACID	334485	1		P	21.00
18	7.36	%BENZENE ACETIC ACID	103822	1		P	16.00
19	7.36	CIS-2,3-DIMETHYLBUTENEDIOIC ACID	488211	1		P	18.00
20	7.36	+ %$1,3-DIMETHYLBENZENE	108383		1	P	10.00
21	7.36	%DIBROMOCHLOROMETHANE	124481		1	P	10.00
22	7.36	%*+$1,4-DICHLOROBENZENE	106467		1	P	1.00
23	7.36	%TRIBROMOMETHANE	75252		1	P	9.00
24	7.36	%1-METHYL-2,4-DINITROBENZENE	121142		1	P	10.00
25	7.36	%*+$NITROBENZENE	98953		1	P	3.00
26	7.36	+ %+NAPHTHALENE	91203		1	P	13.00
27	6.36	%HEXANOIC ACID	142621	1		P	14.00
28	6.36	%*4-METHYL PHENOL	106445	1		T	5.00
29	6.36	2,3,3-TRICHLORO-2-PROPENOIC ACID	2257354	1		T	5.00
30	6.36	%BENZOIC ACID	65850	1		P	130.00
31	6.36	%3-PHENYLPROPIONIC ACID	501520	1		T	5.00
32	6.36	ACETIC ACID, 2-METHYL PHENYL ESTER	533186	1		T	7.00
33	6.36	TETRAMETHYL-1,4-HYDROQUINONE	527184	1		T	5.00
34	6.36	4-ETHYLTETRAMETHYLPHENOL	5081	1		T	5.00
35	6.36	OCTANEDIOIC ACID	505486	1		P	8.00
36	6.36	PHENOXY ACETIC ACID	122598	1		P	8.00
37	6.36	4-(1,5-DIMETHYL-3-OXOHEXYL)-1-CYCLOHEXENE-1-CARBOXYLIC ACID	17844074	1		T	11.00
38	6.36	2-METHOXYBENZOIC ACID	579759	1		P	10.00
39	6.36	12-METHYLTETRADECANOIC ACID	5502943	1		P	3.00
40	6.36	PENTADECANOIC ACID	1002842	1		P	4.00
41	6.36	2-(4-CHLOROPHENOXY)-2-METHYLPROPANOIC ACID	882097	1		P	8.00
42	6.36	%1,2-BENZENEDICARBOXYLIC ACID	88993	1		P	8.00
43	6.36	UNDECANEDIOIC ACID	1852046	1		P	7.00
44	6.36	%*(2,4-DICHLOROPHENOXY)ACETIC ACID	94757	1		T	5.00
45	6.36	+ %$1,2-DIMETHYLBENZENE	95476		1	P	4.00

(continued)

TABLE B11. (continued)

COMPOUNDS FOUND IN CONCENTRATE BY RELATIVE SIZE (PART I)
UNDER FRACTION, 1=FOUND ON GC COLUMN 1, 2=FOUND ON GC COLUMN 2, 3=FOUND ON BOTH GC COLUMN 1 AND GC COLUMN 2
CINCINNATI IV GAC FEED, XAD ETHER ELUATE, WITHOUT SULFITE

SEQ NO.	RS	SYSTEMATIC NAME	CAS NO.	FRACTION		POS. OR TENT ID	CONC. (%HEB)
				2	9		
46	6.36	† 1,2,4-TRIMETHYL BENZENE	95636		1	P	4.00
47	6.36	O-NITROTOLUENE	88722		1	T	1.00
48	6.36	† 4-ETHYL BENZOIC ACID, METHYL ESTER	4346183		1	T	1.00
49	6.36	2,6-DINITROTOLUENE	606202		1	P	5.00
50	6.36	P-CHLORO-2-NITHROANILINE	89634		1	T	3.00
51	6.36	HEXANEDIOIC ACID,DIHEXYL ESTER	110338		1	T	7.00
52	6.36	1,1≠-OXYBIS-OCTANE	629823		1	T	4.00
53	5.36	%CHLOROACETIC ACID	79118	1		P	3.00
54	5.36	%3-METHYLPHENOL	108394	1		P	2.00
55	5.36	4-METHYL-1,2-BENZENEDICARBOXYLIC ACID	4316238	1		P	2.00
56	5.36	4-METHYLBENZOIC ACID	99945	1		P	3.00
57	5.36	%2-HYDROXYBENZOIC ACID	69727	1		P	3.00
58	5.36	%*+PHENOL	108952	1		P	1.50
59	5.36	† $ETHYLBENZENE	100414		1	P	3.00
60	5.36	† %$1,4-DIMETHYBENZENE	106423		1	P	2.00
61	5.36	† %1,3,5-TRIMETHYL BENZENE	108578		1	P	0.50
62	5.36	† 1-ETHYL-3,5-DIMETHYL BENZENE	934747		1	P	11.00
63	5.36	† 1,2,3-TRIMETHYL BENZENE	526738		1	P	2.00
64	5.36	† 2-ETHYL-1,4-DIMETHYL BENZENE	1758889		1	T	1.00
65	5.36	† 1-ETHYL-2,4-DIMETHYL BENZENE	874419		1	P	0.50
66	5.36	† 4-ETHYL-1,2-DIMETHYL BENZENE	934805		1	P	2.00
67	5.36	ETHYL DICHLOROACETATE	535159		1	T	1.00
68	5.36	† 1-ETHENYL-4-ETHYLBENZENE	3454077		1	P	1.50
69	5.36	%BENZALDEHYDE	100527		1	P	1.00
70	5.36	BENZONITRILE	100470		1	P	3.00
71	5.36	† %BENZOIC ACID, ETHYL ESTER	93890		1	P	1.00
72	5.36	† METHYLP-ETHYLBENZOATE	7364207		1	P	1.00
73	5.36	† %2-METHYLNAPHTHALENE	91576		1	P	1.00
74	5.36	P-NITROTOLUENE	99990		1	T	1.00
75	5.36	HEXADECANOIC ACID, METHYL ESTER	112390		1	P	2.00
76	5.36	HEXADECANOIC ACID, ETHYL ESTER	628977		1	P	2.00
77	5.36	OCTADECANOIC ACID, METHYL ESTER	112618		1	P	1.00
78	4.36	%3,4-DICHLOROBENZAMINE	95761		1	T	1.00

† A PROBABLE OR POSSIBLE XAD-2 RESIN BLEED ARTIFACT.

TABLE B12. COMPOUND IDENTIFICATION RESULTS FOR THE CINCINNATI GAC CONTACTOR A SAMPLE, T4Y1, PRE-GAC 10-LITER PERMEATE

COMPOUNDS FOUND IN CONCENTRATE BY RELATIVE SIZE (PART I)
UNDER FRACTION, 1=FOUND ON GC COLUMN 1, 2=FOUND ON GC COLUMN 2, 3=FOUND ON BOTH GC COLUMN 1 AND GC COLUMN 2
CINCINNATI IV GAC FEED, XAD PERMEATE, WITH SULFITE

Code Name T4Y1

SEQ NO.	RS	SYSTEMATIC NAME†	CAS NO.	FRACTION 2	FRACTION 9	POS. OR TENT ID	CONC. (%HEB)
1	8.36	%BENZOIC ACID	65850	1		P	120.00
2	7.36	CIS-?,3-DIMETHYLBUTENEDIOIC ACID	488211	1		P	20.00
3	7.36	CIS-2-ETHYL-3-METHYL-2-BUTENEDIOIC ACID	41654095	1		T	23.00
4	7.36	4-ETHOXYETHYLANILINE	55956291	1		T	10.00
5	6.36	2-ETHYLHEXANOIC ACID	149575	1		P	5.00
6	6.36	DIETHYLENE GLYCOL, MONOMETHYL ETHER	111773	1		P	3.00
7	6.36	N-PHENYL ACETAMIDE	103844	1		T	3.00
8	6.36	3-HYDROXY-1,2-BENZISOTHIAZOLE	27655261	1		T	5.00
9	6.36	%BENZOIC ACID METHYL ESTER	93583		1	P	4.00
10	6.36	† %+NAPHTHALENE	91203		1	P	3.00
11	5.36	%1,2-BENZENEDICARBOXYLIC ACID, MONOBUTYL ESTER	131704	1		P	2.00
12	5.36	%4-METHYL BENZENESULFONAMIDE	70553	1		T	2.00
13	4.36	ISOMYRISTIC ACID	543	1		P	1.00
14	4.36	1,1,1,5,5,5-HEXACHLOROPENTANE	30353594		1	T	0.50

† POSSIBLE XAD-2 RESIN BLEED ARTIFACT.

TABLE B13. COMPOUND IDENTIFICATION RESULTS FOR THE CINCINNATI GAC CONTACTOR A SAMPLE, T4Y3, PRE-GAC 10-LITER XAD-2 PERMEATE

COMPOUNDS FOUND IN CONCENTRATE BY RELATIVE SIZE (PART I)
UNDER FRACTION, 1=FOUND ON GC COLUMN 1, 2=FOUND ON GC COLUMN 2, 3=FOUND ON BOTH GC COLUMN 1 AND GC COLUMN 2
CINCINNATI IV GAC FEED, XAD PERMEATE, WITHOUT SULFITE

Code Name T4Y3

SEQ NO.	RS	SYSTEMATIC NAME †	CAS NO.	FRACTION 2	FRACTION 9	POS. OR TENT ID	CONC. (%HEB)
1	9.36	%BENZOIC ACID	65850	1		P	20.00
2	8.36	10-UNDECENOIC ACID	112389	1		T	40.00
3	8.36	%9-OCTADECENOIC ACID	112801	1		T	92.00
4	8.36	%4-METHYL BENZENESULFONAMIDE	70553	1		T	35.00
5	8.36	3-HEXANONE	589388		1	T	45.00
6	7.36	CIS-2,3-DIMETHYLBUTENEDIOIC ACID	488211	1		P	10.00
7	7.36	CIS-2-ETHYL-3-METHYL-2-BUTENEDIOIC ACID	41654095	1		T	15.00
8	7.36	HEPTADECENOIC ACID	26265396	1		T	15.00
9	7.36	8,11-OCTADECADIENOIC ACID	2197526	1		T	16.00
10	7.36	1,4-BENZOTHIAZIN-3-ONE	5325202	1		T	13.00
11	6.36	ISOMYRISTIC ACID	543	1		P	4.00
12	6.36	3-HYDROXY-1,2-BENZISOTHIAZOLE	27655261	1		T	7.00
13	6.36	ISOPENTADECANOIC ACID	544	1		T	7.00
14	6.36	%BENZOIC ACID METHYL ESTER	93583		1	P	3.50
15	6.36	† %+NAPHTHALENE	91203		1	P	3.50
16	5.36	1,1,1,5,5,5-HEXACHLOROPENTANE	30353594		1	T	3.00
17	4.36	† %8METHYLBENZENE	108883		1	P	0.50
18	4.36	%DIBROMOCHLOROMETHANE	124481		1	P	0.50
19	4.36	%9-METHYLANTHRACENE	779022		1	T	1.00

† POSSIBLE XAD-2 RESIN BLEED ARTIFACT.

APPENDIX C

COMPOUND IDENTIFICATION RESULTS FOR THE SEVEN CINCINNATI GAC CONTACTOR D SAMPLES--COMPUTER-PRINTED TABLES

Appendix C contains the compound identification results for the seven Cincinnati GAC contactor D samples as the separate computer-printed tables for each sample. These individual listings are in decreasing order of the RS values of the GC peaks. Their presentation as separate lists for each sample facilitates the review of the compound identification results of individual samples compared to the use of Table 9 for that purpose. The information provided for each identified compound by these tables which is not available in the combined computer-printed listing of Table 9 includes the following:

- RS values for each identified compound
- Identification status (confirmed, P, and tentative, T) for each identified compound
- The CAS number for each identified compound
- The systematic name of each compound
- The fraction in which each identification was made (acid, aromatic/medium polarity neutrals, or unpartitioned neutrals)

Column headers and symbols used in these computer-printed tables are explained in the section, Abbreviations and Symbols.

TABLE C1. COMPOUND IDENTIFICATION RESULTS FOR THE CINCINNATI GAC CONTACTOR D SAMPLE, T5R4, PRE-GAC 200-FOLD CELLULOSE ACETATE RO BRINE

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COMPOUNDS FOUND IN CONCENTRATE BY RELATIVE SIZE (PART I)
UNDER FRACTION, 1=FOUND ON GC COLUMN 1, 2=FOUND ON GC COLUMN 2, 3=FOUND ON BOTH GC COLUMN 1 AND GC COLUMN 2
CINCINNATI V GAC FEED, 200 X CA RO

Code Name T5R4

SEQ NO.	RS	SYSTEMATIC NAME	CAS NO.	FRACTION 2	FRACTION 4	POS. OR TENT ID	CONC. (%HEB)
1	24.36	%BENZOIC ACID	65850	1		P	20.00
2	9.36	CIS-2-ETHYL-3-METHYL-2-BUTENEDIOIC ACID	41654095	1		T	112.00
3	9.36	%1-PHENYLETHANONE	98862		1	P	119.00
4	9.36	1,3,5-TRIMETHYL-1,3,5-TRIAZINE-2,4,6-TRIONE	827167		1	P	156.00
5	8.36	CIS-2,3-DIMETHYLBUTENEDIOIC ACID	488211	1		P	83.00
6	8.36	10-OXO-UNDECANOIC ACID	676006	1		T	65.00
7	8.36	%7-OXABICYCLO[4.1.0]HEPTANE	286204		1	T	35.00
8	7.36	%BENZENE ACETIC ACID	103822	1		P	18.00
9	7.36	3-HYDROXYNONANOIC ACID	33796871	1		T	30.00
10	7.36	2-(4-CHLOROPHENOXY)-2-METHYLPROPANOIC ACID	882097	1		P	25.00
11	7.36	%DIBROMOCHLOROMETHANE	124481		1	P	14.00
12	7.36	2,5-HEXANEDIONE	110134		1	P	11.00
13	7.36	METHOXY PROPOXY PROPANOL	425		1	P	13.00
14	7.36	TRIMETHYLNAPHTHALENE	311		1	T	11.00
15	7.36	4-HYDROXY-4-METHYLCYCLOHEXANONE	17429026		1	T	10.00
16	6.36	4-OXO-PENTANOIC ACID	123762	1		P	7.00
17	6.36	3-METHYLBENZOIC ACID	99047	1		P	7.00
18	6.36	4-METHYLBENZOIC ACID	99945	1		P	5.00
19	6.36	%2-HYDROXYBENZOIC ACID	69727	1		P	9.00
20	6.36	%3-PHENYLPROPIONIC ACID	501520	1		P	9.00
21	6.36	P-ETHYLBENZOIC ACID	619647	1		P	5.00
22	6.36	3-HYDROXYOCTANOIC ACID	14292274	1		T	10.00
23	6.36	2-METHOXYBENZOIC ACID	579759	1		P	10.00
24	6.36	4-METHOXYBENZOIC ACID	100094	1		P	5.00
25	6.36	%1,2-BENZENEDICARBOXYLIC ACID	88993	1		P	5.00
26	6.36	DIMETHYL-(1-METHYLETHYL)BENZENE	103		1	T	5.00
27	6.36	N,N-DIETHYFORMAMIDE	617845		1	P	9.00
28	6.36	%1,7,7-TRIMETHYLBICYCLO[2.2.1]HEPTAN-2-ONE	76222		1	P	6.00
29	6.36	5,5-DIMETHYL-2(5H)-FURANONE	20019641		1	T	5.00
30	6.36	5,6,7,7A-TETRAHYDRO-4,4,7A-TRIMETHYL-2(4H)-BENZOFURANONE	17092921		1	T	10.00
31	6.36	1-METHYL-9H-FLUORENE	1730376		1	T	4.00
32	6.36	METHOXY PROPOXY PROPANOL	426		1	P	5.00
33	5.36	%TRIBROMOMETHANE	75252		1	P	3.00

TABLE C2. COMPOUND IDENTIFICATION RESULTS FOR THE CINCINNATI GAC CONTACTOR D SAMPLE, T5E1, PRE-GAC, 10-LITERS, NO RO PROCESSING

COMPOUNDS FOUND IN CONCENTRATE BY RELATIVE SIZE (PART I)
UNDER FRACTION, 1=FOUND ON GC COLUMN 1, 2=FOUND ON GC COLUMN 2, 3=FOUND ON BOTH GC COLUMN 1 AND GC COLUMN 2
CINCINNATI V GAC FEED
Code Name T5E1

SEQ NO.	RS	SYSTEMATIC NAME	CAS NO.	FRACTION 2	FRACTION 4	POS. OR TENT ID	CONC. (%HEB)
1	10.36	%BROMODICHLOROMETHANE	75274		1	P	420.00
2	9.36	%BENZOIC ACID	65850	1		P	102.00
3	9.36	%DIBROMOCHLOROMETHANE	124481		1	P	229.00
4	9.36	1,2-DICHLOROCYCLOHEXANE	822866		1	T	168.00
5	9.36	1,3,5-TRIMETHYL-1,3,5-TRIAZINE-2,4,6-TRIONE	827167		1	P	196.00
6	8.36	CIS-2-ETHYL-3-METHYL-2-BUTENEDIOIC ACID	41654095	1		T	55.00
7	8.36	2-ETHYL-4-METHYL-1,3-DIOXOLANE	4359450		1	T	25.00
8	8.36	1-CHLORO-2,4-HEXADIENE	34632896		1	T	36.00
9	8.36	2,6-DIMETHYL-4-HEPTANONE	108838		1	P	44.00
10	8.36	%TRIBROMOMETHANE	75252		1	P	75.00
11	8.36	1,2,3,4-TETRAHYDRONAPHTHALENE	119642		1	P	49.00
12	8.36	2,3-DIHYDRO-1H-INDEN-1-ONE	83330		1	P	37.00
13	8.36	%1,1≠-OXYBISBENZENE	101848		1	P	37.00
14	8.36	%TRIBUTYL PHOSPHATE	126738		1	P	38.00
15	7.36	%HEXANOIC ACID	142621	1		P	20.00
16	7.36	CIS-2,3-DIMETHYLBUTENEDIOIC ACID	488211	1		P	24.00
17	7.36	2-(4-CHLOROPHENOXY)-2-METHYLPROPANOIC ACID	882097	1		P	10.00
18	7.36	%4-METHYL-3-PENTEN-2-ONE	141797		1	T	8.00
19	7.36	%CHLOROBENZENE	108907		1	P	9.00
20	7.36	1,1-DICHLOROCYCLOHEXANE	2108921		1	T	26.00
21	7.36	HEXACHLOROETHANE	67721		1	P	9.00
22	7.36	%+$1,2-DICHLORO BENZENE	95501		1	P	19.00
23	7.36	CIS-1-BROMO-2-CHLOROCYCLOHEXANE	51422754		1	T	29.00
24	7.36	+3,5,5-TRIMETHYL-2-CYCLOHEXEN-1-ONE	78591		1	P	18.00
25	7.36	BENZONITRILE	100470		1	P	16.00
26	7.36	0-NITROTOLUENE	88722		1	T	18.00
27	7.36	%BENZENEACETONITRILE	140294		1	P	14.00
28	7.36	3,4-DIHYDRO-1(2H)-NAPHTHALENONE	529340		1	T	31.00
29	6.36	%HEPTANOIC ACID	111148	1		P	5.00
30	6.36	%DICHLOROACETIC ACID	79436	1		T	3.00
31	6.36	2-METHYL BENZOIC ACID	118901	1		P	5.00
32	6.36	3-METHYLBENZOIC ACID	99047	1		P	2.00
33	6.36	ALPHA-METHYLBENZENEACETIC ACID	492375	1		P	2.00
34	6.36	3-(P-TOLYL)PROPIONIC ACID	7495843	1		T	4.00
35	6.36	%3-PHENYLPROPIONIC ACID	501520	1		P	3.50
36	6.36	2,4-DIMETHYL BENZOIC ACID	611018	1		T	3.00
37	6.36	2-ACETYL-P-TOLUIC ACID	15482549	1		T	3.50
38	6.36	4-PHENYLPENTANOIC ACID	16433435	1		T	7.00
39	6.36	4-METHOXYBENZOIC ACID	100094	1		P	3.00
40	6.36	%[2-(P-CHLOROPHENOXY)-2-METHYL]PROPIONIC ACID	93652	1		T	2.50
41	6.36	4-(1,5-DIMETHYL-3-OXOHEXYL)CYCLOHEXANECARBOXYLIC ACID	38963916	1		T	2.00
42	6.36	%*(2,4-DICHLOROPHENOXY)ACETIC ACID	94757	1		T	3.00
43	6.36	4-CHLOROCYCLOHEXENE	930654		1	T	3.00
44	6.36	CYCLOHEPTANONE	502421		1	T	7.00
45	6.36	2-METHYL-2-CYCLOPENTEN-1-ONE	1120736		1	T	7.00

(continued)

TABLE C2. (continued)

COMPOUNDS FOUND IN CONCENTRATE BY RELATIVE SIZE (PART I)
UNDER FRACTION, 1=FOUND ON GC COLUMN 1, 2=FOUND ON GC COLUMN 2, 3=FOUND ON BOTH GC COLUMN 1 AND GC COLUMN 2
CINCINNATI V GAC FEED
Code Name T5E1

SEQ NO.	RS	SYSTEMATIC NAME	CAS NO.	FRACTION		POS. OR TENT ID	CONC. (%HEB)
				2	4		
46	6.36	DICHLOROACETONITRILE	3018120		1	T	2.00
47	6.36	1,1,3-TRICHLORO-1-PROPENE	2567148		1	T	3.00
48	6.36	%+$1,3-DICHLOROBENZENE	541731		1	P	3.00
49	6.36	3-METHYL-2-CYCLOPENTEN-1-ONE	2758181		1	P	3.00
50	6.36	%+$1,1#-OXYBIS(2-CHLOROETHANE)	111444		1	P	5.00
51	6.36	3-PROPYLCYCLOPENTENE	34067759		1	T	4.00
52	6.36	1,3,3-TRIMETHYLBICYCLO(2.2.1)HEPTAN-2-OL	1632731		1	P	5.00
53	6.36	%PHOSPHORIC ACID, TRIETHYLESTER	78400		1	P	6.00
54	6.36	METHOXYPROPOXY PROPOXY PROPANOL	400		1	P	5.00
55	6.36	METHOXYPROPOXY PROPOXY PROPANOL	401		1	P	9.00
56	6.36	METHOXYPROPOXY PROPOXY PROPANOL	402		1	P	7.00
57	6.36	METHOXYPROPOXY PROPOXY PROPANOL	403		1	P	6.00
58	6.36	1-(1-METHYL-2-(2-PROPENYLOXY)ETHOXY)-2-PROPANOL	55956257		1	T	5.00
59	6.36	1,1,1,5,5,5-HEXACHLOROPENTANE	30353594		1	T	7.00
60	6.36	1,2,3,4-TETRAHYDRO-1-NAPHTHALENOL	529339		1	T	5.00
61	6.36	TETRAHYDRO-1,1-DIOXIDE THIOPHENE	126330		1	P	5.00
62	6.36	N-(4-CHLOROPHENYL)ACETAMIDE	539037		1	T	9.00
63	6.36	5,6,7,7A-TETRAHYDRO-4,4,7A-TRIMETHYL-2(4H)-BENZOFURANONE	17092321		1	T	8.00
64	6.36	1(3H)-ISOBENZOFURANONE	87412		1	P	4.00
65	6.36	%1-METHYL-2,4-DINITROBENZENE	121142		1	P	7.00
66	6.36	%*+$NITROBENZENE	98953		1	P	30.00
67	6.36	DICHLOROBUTENE	110576		1	T	2.00
68	6.36	4-HYDROXY-4-METHYLCYCLOHEXANONE	17429026		1	T	3.00
69	6.36	4-PHENYL-3-BUTEN-2-ONE	122576		1	T	6.00
70	5.36	2,2-DIMETHYLPENTANOIC ACID	1185393	1		T	1.00
71	5.36	2-METHYLCAPRYLIC ACID	3004931	1		T	1.50
72	5.36	DIVINYL MERCURY	1119206	1		T	1.00
73	5.36	3,6-DIMETHYLOCTANOIC ACID	4812297	1		T	2.00
74	5.36	%BENZENE ACETIC ACID	103822	1		P	2.50
75	5.36	%4 CHLOROBENZOIC ACID	74113	1		P	1.00
76	5.36	3-PHENYL PENTANOIC ACID	5669170	1		T	2.00
77	5.36	4-BUTOXYBUTANOIC ACID	55724737	1		T	2.00
78	5.36	%1,2-BENZENEDICARBOXYLIC ACID	88993	1		P	1.50
79	5.36	4-METHYLBENZOIC ACID	99945	1		P	1.50
80	5.36	$2-CHLOROPHENOL	95578	1		T	0.50
81	5.36	N-PHENYL ACETAMIDE	103844		1	T	42.00
82	5.36	%9H-FLUOREN-9-ONE	486259		1	P	1.00

TABLE C3. COMPOUND IDENTIFICATION RESULTS FOR THE CINCINNATI GAC CONTACTOR D SAMPLE, T5G1, POST-GAC, 10-LITERS, NO RO PROCESSING

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COMPOUNDS FOUND IN CONCENTRATE BY RELATIVE SIZE (PART I)
UNDER FRACTION, 1=FOUND ON GC COLUMN 1, 2=FOUND ON GC COLUMN 2, 3=FOUND ON BOTH GC COLUMN 1 AND GC COLUMN 2
CINCINNATI V POST GAC
Code Name T5G1

SEQ NO.	RS	SYSTEMATIC NAME	CAS NO.	FRACTION 2	FRACTION 4	POS. OR TENT ID	CONC. (%HEB)
1	7.36	3-METHOXY-3-METHYL-2-BUTANONE	36687986	1		T	10.00
2	6.36	DIBUTYL SULFITE	626857	1		T	5.00
3	5.36	X*4-METHYL PHENOL	106445	1		P	2.00
4	5.36	BENZOTHIAZOLE	95169		1	P	6.00
5	5.36	1,3,5-TRIMETHYL-1,3,5-TRIAZINE-2,4,6-TRIONE	827167		1	P	1.00

TABLE C4. COMPOUND IDENTIFICATION RESULTS FOR THE CINCINNATI GAC CONTACTOR D SAMPLE, T5Y1, POST-GAC, XAD-2 CONCENTRATE

WATER POLLUTANTS 02/01/81 PAGE 253

COMPOUNDS FOUND IN CONCENTRATE BY RELATIVE SIZE (PART I)
UNDER FRACTION, 1=FOUND ON GC COLUMN 1, 2=FOUND ON GC COLUMN 2, 3=FOUND ON BOTH GC COLUMN 1 AND GC COLUMN 2
CINCINNATI V POST GAC, XAD ETHER ELUATE

Code Name T5Y1

SEQ NO.	RS	SYSTEMATIC NAME†	CAS NO.	FRACTION 2	FRACTION 4	POS. OR TENT ID	CONC. (%HEB)
1	11.36	† 1-ETHENYL-4-ETHYLBENZENE	3454077	1	1	P	1280.00
2	11.36	† 1,3-DIETHYL BENZENE	141935		1	P	990.00
3	11.36	† 1-ETHENYL-3-ETHYLBENZENE	7525624		1	T	1160.00
4	11.36	† 2,3-DIHYDRO-5-METHYL-1H-INDENE	874351		1	P	1110.00
5	10.36	† 1-ETHYL-3-METHYL BENZENE	620144		1	P	480.00
6	10.36	† 1,4-DIETHYL BENZENE	105055		1	P	970.00
7	10.36	† 1,2-DIETHYL BENZENE	135013		1	P	475.00
8	10.36	† DIETHYL METHYL BENZENE	25550134		1	T	670.00
9	10.36	† 1-ETHYL-4-(1-METHYLETHYL)BENZENE	4218488		1	T	325.00
10	10.36	† 2,3-DIHYDRO-1-METHYL-1H-INDENE	767588		1	T	465.00
11	10.36	† 2,4,6-TRIMETHYLSTYRENE	769255		1	P	350.00
12	10.36	† DIETHENYLBENZENE	1321740		1	T	480.00
13	10.36	† 1,3-DIETHENYLBENZENE	108576		1	T	360.00
14	10.36	†%BENZOIC ACID METHYL ESTER	93583		1	P	575.00
15	9.36	†%$(1-METHYL ETHYL) BENZENE	98828		1	P	1090.00
16	9.36	† 2-METHYLDECALIN	2958761		1	T	145.00
17	9.36	† 1-ETHYL-4-METHYL BENZENE	622968		1	P	270.00
18	9.36	† ETHYLDECALIN	25551499		1	T	120.00
19	9.36	† 1-ETHENYL-2-ETHYLBENZENE	7564638		1	T	275.00
20	9.36	† 2,4-DIMETHYL-1-(1-METHYLPROPYL)BENZENE	1483609		1	T	110.00
21	9.36	† 2-METHYL-2, 3-DIHYDRO-1H-INDENE	824635		1	T	140.00
22	9.36	† 4-METHYL-2,3 DIHYDRO-1H-INDENE	824226		1	T	190.00
23	9.36	† 1,2,3,4-TETRAHYDRONAPHTHALENE	119642		1	P	225.00
24	9.36	† A PENTENYLBENZENE	5080		1	T	180.00
25	9.36	† 1,1A,6,6A-TETRAHYDROCYCLOPROP(A)INDENE	15677153		1	T	135.00
26	9.36	HEXANEDIOIC ACID,DIHEXYL ESTER	110338		1	T	265.00
27	8.44	† HEXADECANOIC ACID, ETHYL ESTER	628977	1	1	P	7.00
28	8.36	† %$1,3-DIMETHYLBENZENE	108383	1		P	68.00
29	8.36	%BENZOIC ACID	65850	1		P	63.00
30	8.36	3-METHOXY-3-METHYL-2-BUTANONE	36687986		1	T	40.00
31	8.36	† (1-METHYLPROPYL) BENZENE	135988		1	P	45.00
32	8.36	† (1,1-DIMETHYLPROPYL)BENZENE	2049958		1	T	30.00
33	8.36	† 4-ETHYL-1,2-DIMETHYL BENZENE	934805		1	P	25.00
34	8.36	† 1-PROPENYLBENZENE	637503		1	P	40.00
35	8.36	† (1-ETHYL-2-PROPENYL)-BENZENE	19947229		1	T	40.00
36	8.36	†%BENZOIC ACID, ETHYL ESTER	93890		1	P	85.00
37	8.36	†%1-PHENYLETHANONE	98862		1	P	65.00
38	8.36	† ETHYLBENZALDEHYDE (ISOMER UNKNOWN)	53951501		1	T	90.00
39	8.36	† 4-ETHYL BENZOIC ACID, METHYL ESTER	4346183		1	P	40.00
40	8.36	† 1-(2-ETHYLPHENYL)ETHANONE	2142645		1	T	45.00
41	8.36	†%2-METHYLNAPHTHALENE	91576		1	P	60.00
42	8.36	†%1-METHYLNAPHTHALENE	90120		1	P	50.00
43	8.36	1,5-BIS(T-BUTYL)-3,3-DIMETHYL BICYCLO(3.1.0)HEXAN-2-ONE	1977958		1	T	40.00
44	8.36	† OCTADECANOIC ACID, ETHYL ESTER	111615		1	P	35.00
45	7.60	† TETRADECANOIC ACID, ETHYL ESTER	124061	1	1	P	4.00

(continued)

TABLE C4. (continued)

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COMPOUNDS FOUND IN CONCENTRATE BY RELATIVE SIZE (PART I)
UNDER FRACTION, 1=FOUND ON GC COLUMN 1, 2=FOUND ON GC COLUMN 2, 3=FOUND ON BOTH GC COLUMN 1 AND GC COLUMN 2
CINCINNATI V POST GAC, XAD ETHER ELUATE

Code Name T5Y1

SEQ NO.	RS	SYSTEMATIC NAME†	CAS NO.	FRACTION 2	FRACTION 4	POS. OR TENT ID	CONC. (%HEB)
46	7.36	† $ETHYLBENZENE	100414	1		P	29.00
47	7.36	† %$1,4-DIMETHYBENZENE	106423	1		P	24.00
48	7.36	4-METHYL-2-PENTANOL	108112	1		T	15.00
49	7.36	† %$1,2-DIMETHYLBENZENE	95476	1		P	33.00
50	7.36	2-HEPTANONE	110430	1		T	23.00
51	7.36	2-METHOXYETHANOL	109864	1		T	18.00
52	7.36	1,2-BUTANEDIOL	584032	1		T	17.00
53	7.36	† O-ETHYLBENZOIC ACID	28134318	1		T	16.00
54	7.36	† CYCLOPROPYLBENZENE	873494		1	T	20.00
55	7.36	† METHYL-(2-METHYLPROPYL) BENZENE	100		1	T	10.00
56	7.36	† 1,3,5-TRIETHYLBENZENE	102250		1	P	25.00
57	7.36	† 2-ETHYL-1,2,3,4-TETRAHYDRONAPHTHALENE	32367547		1	T	25.00
58	7.36	N,N-DIETHYL-4-METHYL-2-PENTANAMINE	16627353		1	T	15.00
59	7.36	1-PHENYL-3-BUTEN-2-ONE	37442550		1	T	15.00
60	7.36	† %1-(4-ETHYLPHENYL)ETHANONE	937304		1	P	15.00
61	7.36	† %2-ETHYL NAPHTHALENE	939275		1	P	15.00
62	6.36	%DECANOIC ACID	334485	1		P	6.00
63	6.36	† P-ETHYLBENZOIC ACID	619647	1		P	7.00
64	6.36	† DODECANOIC ACID, ETHYL ESTER	106332	1		P	6.00
65	6.36	4-HYDROXYACETOPHENONE	7339879	1		T	4.00
66	6.36	%NONANEDIOIC ACID	123999	1		P	7.00
67	6.36	%1,2-BENZENEDICARBOXYLIC ACID	88993	1		P	7.00
68	6.36	%1,2-BENZENEDICARBOXYLIC ACID, MONOBUTYL ESTER	131704	1		P	5.00
69	5.36	%OCTANOIC ACID	124072	1		P	3.00
70	5.36	%3-METHYLPHENOL	108394	1		P	2.00
71	5.36	3,4-DIMETHYLPHENOL	95658	1		T	1.00
72	5.36	DIETHYLENE GLYCOL, MONOMETHYL ETHER	111773	1		T	2.00
73	5.36	1,1≠-OXYBIS-2-PROPANOL	110985	1		P	1.00
74	5.36	METHOXY TOLUIC ACID	1701775	1		T	1.50
75	5.36	2-METHOXYBENZOIC ACID	579759	1		P	1.50
76	5.36	1,3-DIOXALANE METHANOL	5694688	1		T	3.00

† A PROBABLE OR POSSIBLE XAD-2 RESIN BLEED ARTIFACT.

TABLE C5. COMPOUND IDENTIFICATION RESULTS FOR THE CINCINNATI GAC CONTACTOR D SAMPLE, T5R1, POST-GAC, 10-FOLD CELLULOSE ACETATE RO BRINE

WATER POLLUTANTS 02/01/81 PAGE 288

COMPOUNDS FOUND IN CONCENTRATE BY RELATIVE SIZE (PART I)
UNDER FRACTION, 1=FOUND ON GC COLUMN 1, 2=FOUND ON GC COLUMN 2, 3=FOUND ON BOTH GC COLUMN 1 AND GC COLUMN 2
CINCINNATI V POST GAC, 10 X CA RO

Code Name T5R1

SEQ NO.	RS	SYSTEMATIC NAME	CAS NO.	FRACTION 2	FRACTION 4	POS. OR TENT ID	CONC. (%HEB)
1	7.36	2-METHYL-3-HEXANONE	7379126	1		T	29.00
2	7.36	3-METHOXYPENTANE	36839675	1		T	11.00
3	7.36	5-HEXYLDIHYDROFURANONE	706149		1	T	13.00
4	6.36	2-ETHYLHEXANOIC ACID	149575	1		P	7.00
5	6.36	%ACETIC ACID, ETHYL ESTER	141786	1		T	5.00
6	6.36	1,3-DIMETHYL-2-(2-ISOPROPYLPHENYL)ETHYLCYCLOHEXANE CARBOXILIC ACID	6080	1		T	8.00
7	6.36	%PHOSPHORIC ACID, TRIETHYLESTER	78400		1	P	3.00
8	6.36	BENZOTHIAZOLE	95169		1	P	12.00
9	6.36	4-(1,1,3,3-TETRAMETHYLBUTYL)PHENOL	140669		1	P	4.00
10	6.36	4-(1-METHYLOCTYL)PHENOL	17404669		1	P	4.00
11	6.36	2-NONENAL	2463538		1	T	6.00
12	6.36	CYCLIC TETRAMETHYLENE ADIPATE	777957		1	T	10.00
13	6.36	%+NAPHTHALENE	91203		1	P	8.00
14	5.36	2-METHYL BENZOIC ACID	118901	1		T	2.00
15	5.36	%1,7,7-TRIMETHYLBICYCLO[2.2.1]HEPTAN-2-ONE	76222		1	P	3.00
16	4.36	1(3H)-ISOBENZOFURANONE	87412	1		P	1.00
17	4.36	%*+$1,4-DICHLOROBENZENE	106467		1	P	1.00
18	4.36	%2-FURANCARBOXALDEHYDE	98011		1	P	1.00

TABLE C6. COMPOUND IDENTIFICATION RESULTS FOR THE CINCINNATI GAC CONTACTOR D SAMPLE, T5R3, POST-GAC, 200-FOLD CELLULOSE ACETATE RO BRINE

WATER POLLUTANTS 02/01/81 PAGE 340

COMPOUNDS FOUND IN CONCENTRATE BY RELATIVE SIZE (PART I)
UNDER FRACTION, 1=FOUND ON GC COLUMN 1, 2=FOUND ON GC COLUMN 2, 3=FOUND ON BOTH GC COLUMN 1 AND GC COLUMN 2
CINCINNATI V POST GAC, 200 X CA RO

Code Name T5R3

SEQ NO.	RS	SYSTEMATIC NAME	CAS NO.	FRACTION 2	FRACTION 4	POS. OR TENT ID	CONC. (%HEB)
1	7.36	DIMETHYL-(1-METHYLETHYL)BENZENE	104		1	T	10.00
2	7.36	CYCLIC TETRAMETHYLENE ADIPATE	777957		1	T	9.00
3	6.36	CIS-1,3-DICHLOROCYCLOHEXANE	24955633		1	T	3.00
4	6.36	%$1,2-BENZENEDICARBOXYLIC ACID, DIMETHYL ESTER	131113		1	P	2.00
5	6.36	2,6-BIS(1,1-DIMETHYL ETHYL)-4-ETHYL PHENOL	4130421		1	T	5.00
6	6.36	%7-OXABICYCLO(4.1.0)HEPTANE	286204		1	T	8.50
7	5.36	DIMETHYL-(1-METHYLETHYL)BENZENE	103		1	T	1.50
8	5.36	%1-PHENYLETHANONE	98862		1	P	1.50
9	5.36	DIMETHYL-(1-METHYLETHYL)BENZENE	105		1	T	1.50
10	5.36	%+$1,2-DICHLORO BENZENE	95501		1	P	2.50
11	5.36	%PHOSPHORIC ACID, TRIETHYLESTER	78400		1	P	2.00
12	5.36	%2,3-DIPHENYLOXIRANE	17619975		1	T	2.00

TABLE C7. COMPOUND IDENTIFICATION RESULTS FOR THE CINCINNATI GAC CONTACTOR D SAMPLE, T5R2, POST-GAC, 10-FOLD NYLON RO BRINE

WATER POLLUTANTS 02/01/81 PAGE 316

COMPOUNDS FOUND IN CONCENTRATE BY RELATIVE SIZE (PART I)
UNDER FRACTION, 1=FOUND ON GC COLUMN 1, 2=FOUND ON GC COLUMN 2, 3=FOUND ON BOTH GC COLUMN 1 AND GC COLUMN 2
CINCINNATI V POST GAC, 10 X NYL RO

Code Name T5R2

SEQ NO.	RS	SYSTEMATIC NAME	CAS NO.	FRACTION 2	FRACTION 4	POS. OR TENT ID	CONC. (%HEB)
1	7.36	%HEXANOIC ACID	142621	1		P	24.00
2	7.36	%HEPTANOIC ACID	111148	1		P	7.00
3	6.36	2-ETHYLHEXANOIC ACID	149575	1		P	10.00
4	6.36	1,3-DIMETHYL-2-(2-ISOPROPYLPHENYL)ETHYLCYCLOHEXANE CARBOXILIC ACID	6880	1		T	7.00
5	6.36	LEVOPIMARIC ACID	79549	1		T	3.00
6	6.36	%+NAPHTHALENE	91203		1	P	7.00
7	6.36	NONYLPHENOL	25154523		1	T	6.00
8	5.36	ISOPIMARIC ACID	5835267	1		T	4.00

APPENDIX D

ANALYSIS RESULTS FOR THE REAGENT WATER SAMPLES--LABELED GC-MS CHROMATOGRAMS

Appendix D contains labeled GC-MS chromatograms for analysis of the unpartitioned aliquot, acid fraction and neutral fraction for the Super-Q reagent water samples. Each chromatogram is accompanied by a table immediately following it in which, for each labeled peak in the chromatogram, the mass spectral data interpretation results are given.

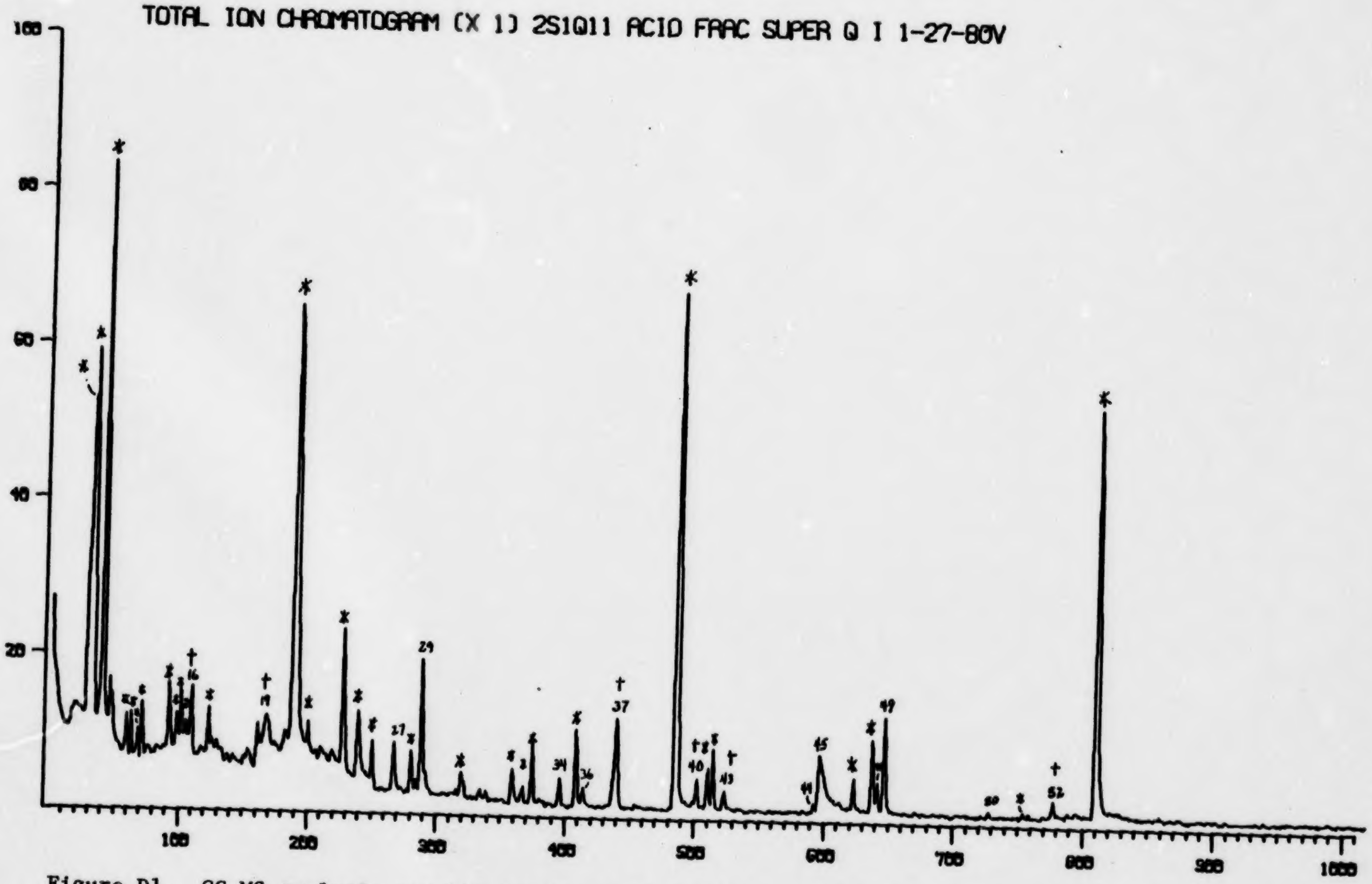

Figure D1. GC-MS analysis results for the acid fraction of the 10-liter reagent water sample, S1Q.

(continued)

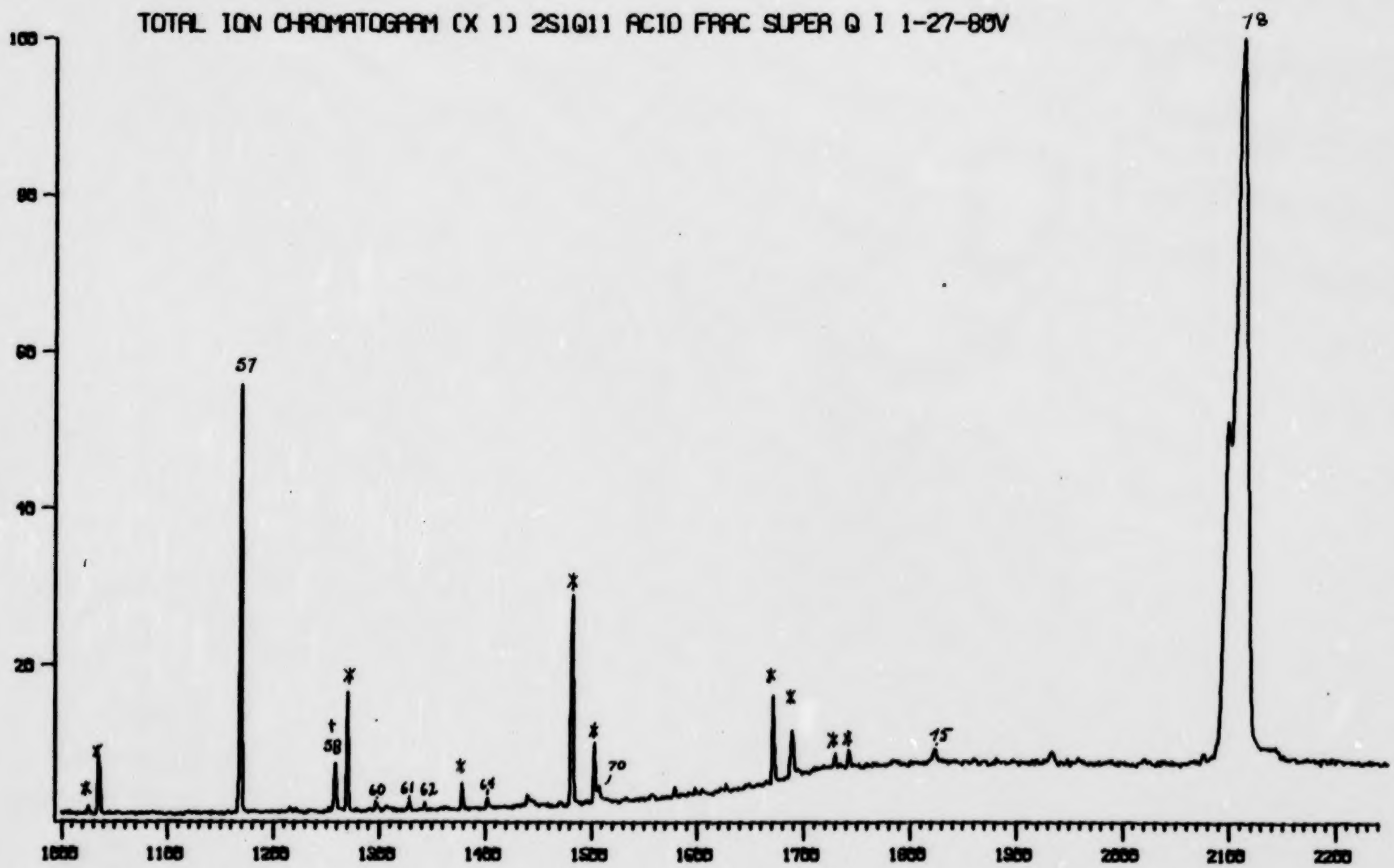

Figure D1. (Continued)

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TABLE D1. GC-MS ANALYSIS RESULTS FOR THE ACID FRACTION OF THE 10-LITER REAGENT WATER SAMPLE, S1Q

Sequence[a]	Spectrum Number	RT	RRT	Compound Name[b]	Molecular Formula	Molecular Weight	GC Peak[c] Size %	IS	RS	Match[d]	Proof[e]
16	109-107	11.843	0.182	†1,4-dioxane	C4.H8.O2	88	16	3		959	B
19	168-164	15.008	0.231	†p-xylene	C8.H10	106	13	2		985	A
27	267-263	20.110	0.309	2-methoxy-1-propanol	C4.J10.O2	90	12	3		992	B
29	288-286	21.183	0.326	2-ethoxyethanol (carbitol impurity?)	C4.H10.O2	90	32	3		934	B
34	396-393	26.641	0.410	BP 45; an alcohol or ether			7	2			
36	414-412	27.545	0.424	propylene glycol			4	2			
37	439-434	28.803	0.443	†phenol, ME-D5, IS + DO, 1:5	C6.H6.O	94	22	3		998	A
40	501-500	31.901	0.491	†octanoic acid, ME	C8.H16.O2	144	7	2		966	A
43	523-519	33.001	0.508	†2-butoxyethanol	C6.H14.O2	118	5	2		977	B
44	592-590	36.435	0.561	1-heptanol	C7.H16.O1	116	3	1		950	A
45	596-593	36.633	0.564	acetic acid (free acid, artifact)	C2.H4.O2	60	14	3		897	A
48	641-640	38.871	0.598	nonanoic acid, ME	C9.H18.O2	158	7	2		963	A
49	647-644	39.171	0.603	isomer of 2-ethyl-1-hexanol	C8.H18.O	130	22.5	3			
50	728-726	43.186	0.664	1-octanol	C8.H18.O	130	2	1		956	A
52	777-775	45.610	0.702	†decanoic acid, ME	C10.H20.O2	172	4	2		man	A
57	1169-1164	64.986	1.000	hexaethylbenzene, IS							
58	1259-1253	69.495	1.069	†phenol + phenol, D5; 20:1	C6.H6.O	94	12	3		996	A
60	1297-1294	71.408	1.099	an unsaturated fatty acid, ME			2	1			
61	1328-1324	72.968	1.123	2,5-dimethylbenzenebutanoic acid, ME	C13.H18.O2	206	3	1		908	B
62	1343-1341	73.726	1.134	anteisopentadecanoic acid, ME	C15.H30.O2	242	2	1		865	A
64	1402-1400	76.710	1.180	an unsaturated fatty acid, ME			3	1			
70	1507-1511	82.110	1.263	1-pentadecanol; a fatty alcohol	C15.H32.O1	228	5	1		man	B
75	1823-1816	98.940	1.522	a fatty alcohol							
78	2115-2102	114.770	1.766	p-methylbenzenesulfonamide, ME, partially in the blank (soap artifact ?)							

---

a) The sequence number is used to label the peaks in the GC-MS chromatogram, Figure D1.

b) ME = methyl ester or methyl ether; IS = internal standard; † = a compound attributable to the 10-liter extraction blank.

c) Size (height) of the GC peak in the GC-MS chromatogram (see a, above) expressed as: %HEB, a percentage of the internal standard, hexaethyl benzene; RS, the relative size parameter explained in Section 5.

d) The quality index of the computer mass spectral library match (Finnigan INCOS software) where the value 1000 reflects a perfect fit of the data mass spectrum with the library mass spectrum.

e) Proof reflects the confidence level of the analyst: A, confirmed identification by comparison to data from a standard; B, highest confidence level for non-confirmable compounds; C, less than 80% confidence level; D, less than 50% confidence level.

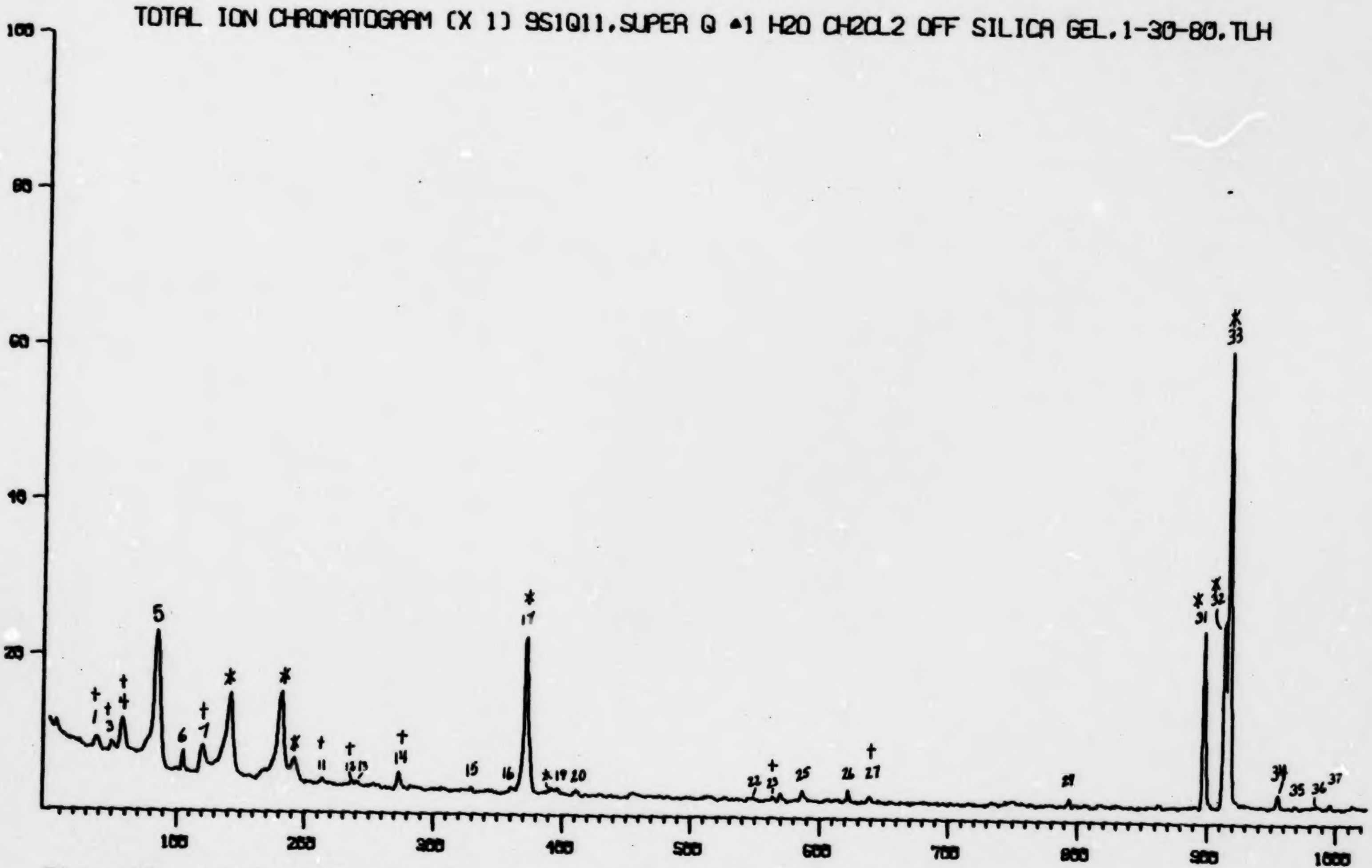

Figure D2. GC-MS analysis results for the aromatic/medium polarity fraction of the 10-liter reagent water sample, S1Q.

(continued)

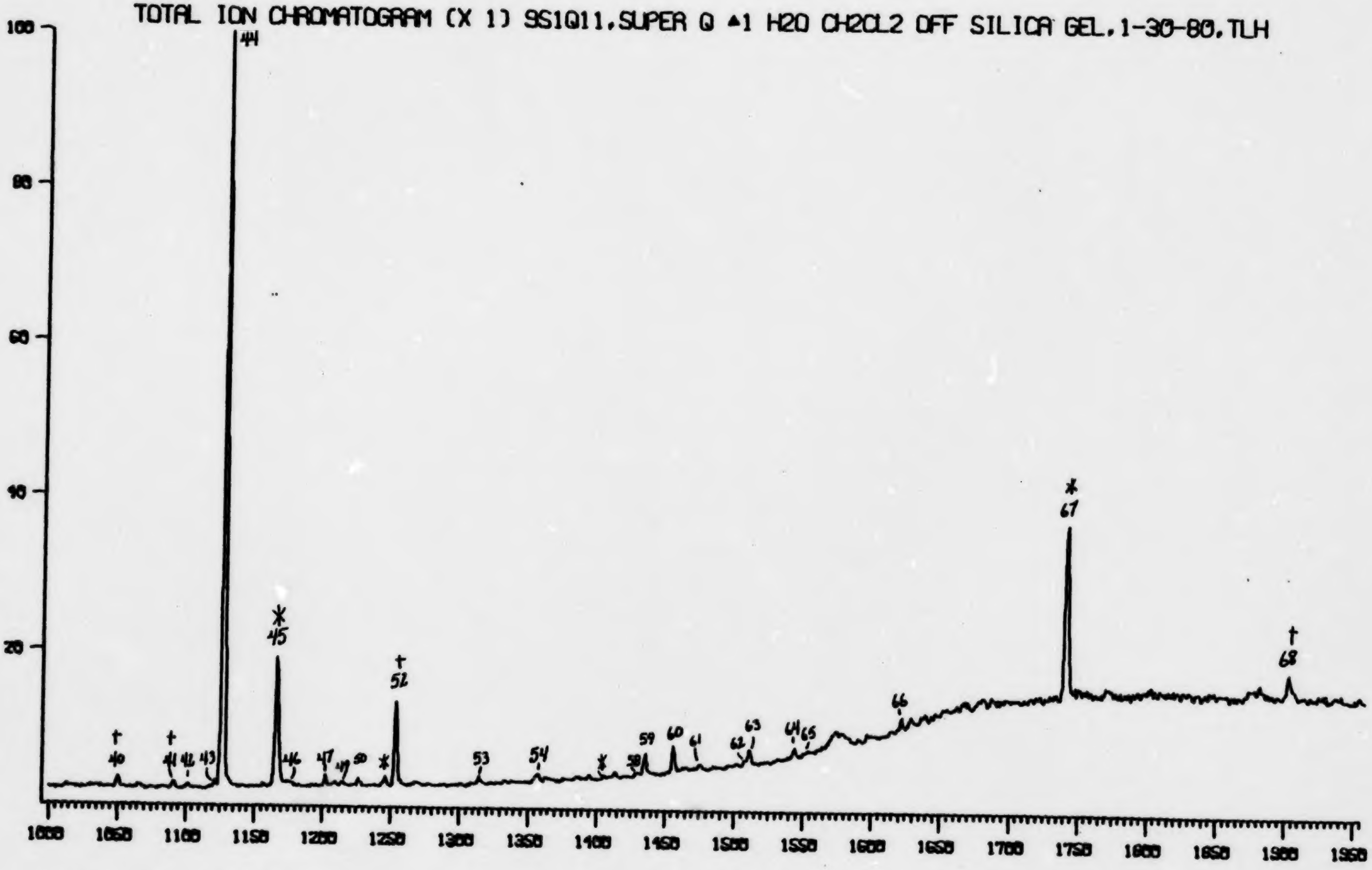

Figure D2. (Continued)

TABLE D2. GC-MS ANALYSIS RESULTS FOR THE AROMATIC/MEDIUM POLARITY FRACTION OF THE 10-LITER REAGENT WATER SAMPLE, S1Q

Sequence[a]	Spectrum Number	RT	RRT	Compound Name[b]	Molecular Formula	Molecular Weight	GC Peak[c] Size		Match[d]	Proof[e]
							% IS	RS		
1	38-33	10.008	0.154	†ethylbenzene	C8.H10	106	1.8	1	995	A
3	50-44	10.641	0.164	†p-xylene	C8.H10	106	1	1	996	A
4	58-53	11.063	0.170	†m-xylene	C8.H10	106	4	2	994	A
5	84-74	12.423	0.191	a hydrocarbon			20	3		
6	105-102	13.520	0.208	a siloxane			3	1		
7	120-114	14.295	0.220	†o-xylene	C8.H10	106	4	2	992	A
11	213-208	19.066	0.293	†mesitylene	C9.H12	120	1	0	963	A
12	236-230	20.238	0.311	†styrene	C8.H8	104	0.5	0	984	B
13	241-245	20.493	0.315	1-ethyl-2-methyl benzene	C9.H12	120	0.5	0	968	A
14	273-268	22.115	0.340	†1,2,4-trimethyl benzene	C9.H12	120	2.5	1	993	A
15	329-333	24.935	0.384	a siloxane			0.5	0		
16	360-355	26.485	0.407	1,2,3-trimethyl benzene	C9.H12	120	1	0	981	A
17	372-364	27.096	0.417	bromobenzene - D5, IS			21			
19	397-400	28.356	0.436	1,3-dimethyl-4-ethyl benzene	C10.H14	134	0.8	0	779	C
20	410-406	29.008	0.446	1,2-dimethyl-4-ethyl benzene	C10.H14	134	1	0	872	C
22	548-545	35.853	0.552	a siloxane			0.5	0		
23	563-557	36.591	0.563	†2-cyclohexen-1-ol	C6.H10.O	98	0.8	0	935	C
25	586-584	37.728	0.580	butyl chloroacetate	C6.H11.O2.CL	150	1.2	1	976	B
26	622-620	39.508	0.608	1,1,2,2-tetrachloroethane	C2.H2.CL4	166	1.2	1	968	B
27	639-635	40.346	0.621	†benzaldehyde	C7.H6.O	106	1	0	985	A
29	794-790	47.978	0.738	1,2,4-trichlorobenzene	C6.H3.CL3	180	1.2	1	995	A
31	898-893	53.113	0.817	dibromobenzene - D4, IS			24			
32	914-909	53.920	0.830	nitrobenzene - D5, IS			25			
33	917-915	54.075	0.832	naphthalene - D8, IS + D0; 5:1			61			
34	955-951	55.975	0.861	2,4,6-cycloheptatrien-1-one	C7.H6.O	106	2	1	990	C
35	968-965	56.620	0.871	1,2,3,5-tetrachlorobenzene	C6.H2.CL4	214	0.5	0	873	A
36	986-989	57.518	0.885	an alkane			0.5	0		
37	996-991	58.016	0.893	methyl laurate	C13.H26.O2	214	1	0	man	B
40	1050-1047	60.710	0.934	†2-methyl naphthalene	C11.H10	142	1.5	1	984	A
41	1091-1095	62.758	0.966	†1-methyl naphthalene	C11.H10	142	1	0	950	A
42	1101-1098	63.256	0.973	an alkane			0.5	0		
43	1122-1118	64.301	0.989	2,6-di-T-butyl-p-cresol (BHT)	C15.H24.O	220	1.2	0	956	A
44	1127-1123	64.576	1.000	hexaethylbenzene, IS						

(continued)

TABLE D2. (continued)

Sequence[a]	Spectrum Number	RT	RRT	Compound Name[b]	Molecular Formula	Molecular Weight	GC Peak[c] Size % IS	RS	Match[d]	Proof[e]
45	1166-1161	66.561	1.031	n-eicosane - D42, IS			17			
46	1174-1177	66.975	1.037	2,6-dimethylnaphthalene	C12.H12	156	1	0	973	A
47	1202-1199	68.386	1.059	biphenyl	C12.H10	154	1.5	1	990	A
49	1214-1212	68.996	1.068	1,6-dimethyl naphthalene plus	C12.H12	156	0.2	0	964	A
				phenol	C6.H6.O1	94	0.2	0		A
50	1226-1223	69.603	1.077	methyl myristate	C15.H30.O2	242	1	0	847	A
52	1253-1250	70.973	1.098	†myristic acid (a fatty acid)	C14.H28.O2	228	11	3	959	D
53	1314-1310	74.075	1.146	a branched alkane			1	1		
54	1357-1352	76.271	1.180	acenaphthene	C12.H10	154	1.5	1	985	A
58	1429-1426	79.981	1.237	2,3-dihydro-1,1,3-trimethyl-3-phenyl-1H-indane	C18.H20	236	0.8	0	847	C
61	1475-1473	82.385	1.274	dibenzofuran	C12.H8.O	168	1	0	978	A
62	1508-1504	84.113	1.301	an alcohol			2	0		
63	1511-1504	84.271	1.303	a fatty alcohol			0.2	1		
64	1544-1541	86.013	1.330	fluorene	C13.H10	166	1.5	1	954	A
65	1554-1549	86.545	1.338	an alcohol			0.8	0		
66	1622-1619	90.203	1.394	methyl stearate	C19.H38.O2	298	1.5	1		A
67	1742-1737	96.800	1.496	1-nitronaphthalene - D7, IS			23			
68	1903-1897	105.690	1.633	†phenanthrene	C14.H10	178	3.5	1	986	A

a) The sequence number is used to label the peaks in the GC-MS chromatogram, Figure D2.

b) ME = methyl ester or methyl ether; IS = internal standard; † = a compound attributable to the 10-liter extraction blank.

c) Size (height) of the GC peak in the GC-MS chromatogram (see a, above) expressed as: %HEB, a percentage of the internal standard, hexaethyl benzene; RS, the relative size parameter explained in Section 5.

d) The quality index of the computer mass spectral library match (Finnigan INCOS software) where the value 1000 reflects a perfect fit of the data mass spectrum with the library mass spectrum.

e) Proof reflects the confidence level of the analyst: A, confirmed identification by comparison to data from a standard; B, highest confidence level for non-confirmable compounds; C, less than 80% confidence level; D, less than 50% confidence level.

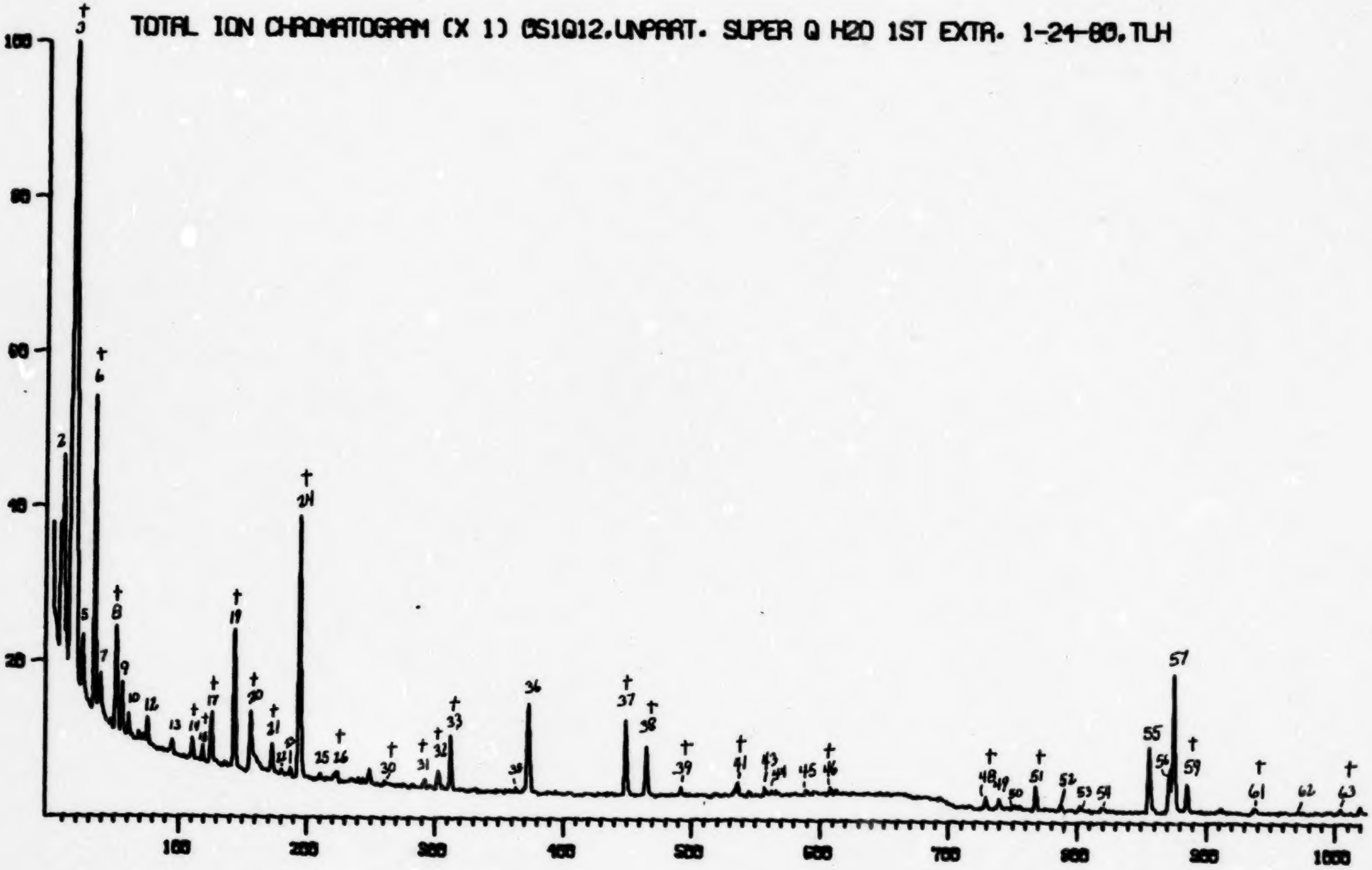

Figure D3. GC-MS analysis results for the unpartitioned aliquot of the 10-liter reagent water sample, S1Q.

(continued)

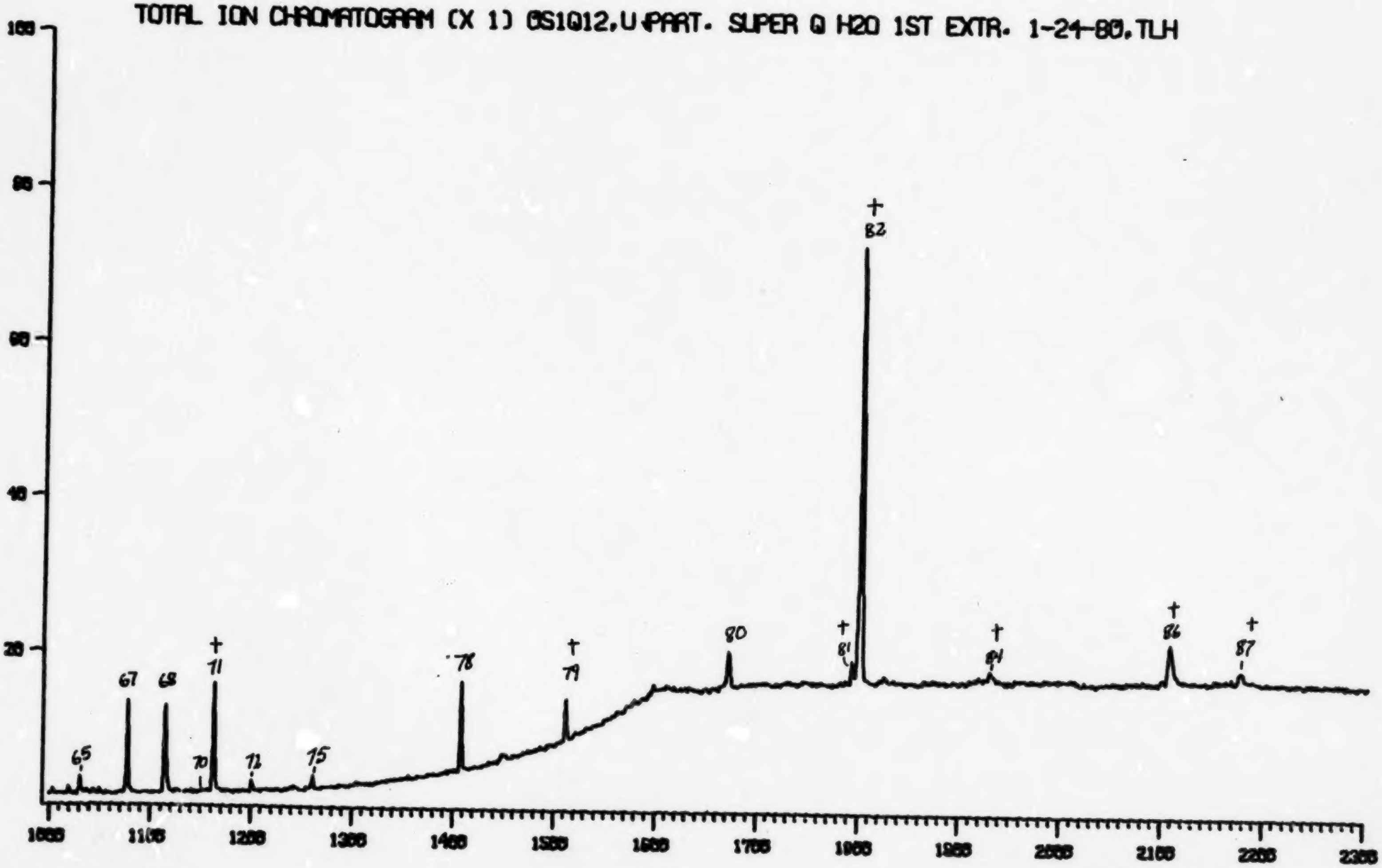
TOTAL ION CHROMATOGRAM (X 1) 0S1Q12,U-PART. SUPER Q H2O 1ST EXTR. 1-24-80,TLH

Figure D3. (Continued)

TABLE D3. GC-MS ANALYSIS RESULTS FOR THE UNPARTITIONED ALIQUOT OF THE 10-LITER REAGENT WATER SAMPLE, S1Q

Sequence[a]	Spectrum Number	RT	RRT	Compound Name[b]	MW	%IS[c]	Relative Retention Times[d]	
							2S1Q11	9S1Q11
2	10-6	9.643	0.145	4-methyl-2-pentanone	100	222		
3	15-13	9.935	0.149	†chloroform	118	683		
5	25-22	10.506	0.158	2-butyne	54	80		
6	34-31	11.016	0.165	†toluene	92	327		
7	39-36	11.301	0.170	bromochloromethane (solvent artifact?)	128	52		
8	51-49	11.981	0.180	†1,4-dioxane	88	112	.182	
9	56-53	12.265	0.184	1,2-dichloroethane	98	56		
10	61-59	12.545	0.188	butyl acetate	116	27		
12	76-74	13.383	0.201	an alkane		30		
13	95-92	14.443	0.217	a siloxane		17		
14	111-107	15.335	0.230	†ethyl benzene	106	25		.154
15	119-116	15.771	0.237	†p-xylene	106	20	.231	.164
17	126-123	16.153	0.242	†m-xylene	106	53		.170
19	144-140	17.135	0.257	†BP 41; m/e 97, 83, 69, 54; a hydrocarbon		144		.191
20	156-154	17.781	0.267	†cyclopentane carboxaldehyde	98	65		
21	173-171	18.701	0.281	†o-xylene	106	31		.220
22	180-178	19.078	0.286	an alkane		8		
23	187-184	19.455	0.292	1,7,7-trimethylbicyclo[2.2.1]hept-2-ene	136	12		
24	194-190	19.830	0.297	†(chloromethyl)oxirane	92	271		
25	210-209	20.681	0.310	1-chloro-2-propanone	92	11		
26	223-219	21.375	0.321	†3-chlorocyclohexene	116	14		
30	261-263	23.383	0.351	†styrene	104	5		.311
31	292-289	25.010	0.375	†1,2,4-trimethylbenzene	120	10		.340
32	302-299	25.535	0.383	†cyclohexanone	98	23		
33	312-310	26.056	0.391	†diethylene glycol, acetate	132	57		
35	362-359	28.658	0.430	1,2,3-trimethyl benzene plus	120	3		.407
				1-methyl-2-propylbenzene	134	3		
36	373-955	29.233	0.438	bromobenzene - D5, IS		91		.417
37	449-445	33.160	0.497	†ethylene glycol, monobutyl ether	118	80	(.508)	
38	465-460	33.983	0.510	†chloroacetonitrile	75	53		
39	492-490	35.373	0.531	†cyclohexen-1-one	96	10		
41	535-531	37.580	0.564	†2-cyclohexen-1-ol	98	17		.563
43	557-554	38.703	0.581	butyl chloroacetate		12		.580
44	562-560	38.960	0.584	2-ethyl-1-hexanol	130	5	(.584)	

(continued)

TABLE D3. (continued)

Sequence[a]	Spectrum Number	RT	RRT	Compound Name[b]	MW	%IS[c]	Relative Retention Times[d] 2S1Q11	9S1Q11
45	589-587	40.343	0.605	1,1,2,2-tetrachloroethane	166	9		.608
46	608-605	41.318	0.620	†benzaldehyde	106	12		.621
48	729-726	47.465	0.712	†diethyl glycol monoethyl ether	134	15		
49	739-737	47.971	0.720	dihydro-2-furanone	86	14		
50	751-746	48.580	0.729	5-methyl-2-(isopropyl)cyclohexanol	156	6		
51	768-764	49.448	0.742	†trans-4-chlorocyclohexanol	134	26		
52	787-785	50.413	0.756	1-chlorodecane	176	4		
53	802-799	51.173	0.768	2-hydroxybenzaldehyde	122	10		
54	819-817	52.035	0.781	branched alkane		8		
55	856-853	53.911	0.809	dibromobenzene - D4, IS		69		.817
56	872-868	54.733	0.821	nitrobenzene - D5, IS		50		.830
57	874-867	54.838	0.823	naphthalene - D8, IS, + D0; 10:1		145		.832
59	885-882	55.408	0.831	†1,3-dichloro-2-propanol	128	29		
61	938-933	58.105	0.872	†diethylene glycol, monobutyl ether	162	12	(.890)	
62	972-966	59.828	0.897	2,3-dichloro-1-propanol	128	4		
63	1004-1000	61.455	0.922	†2-methyl naphthalene	142	8		.934
65	1031-1028	62.835	0.943	2-butyl tetrahydrofuran	128	19		
67	1077-1074	65.195	1.000	hexaethylbenzene, IS		100		
68	1113-1110	67.058	1.028	n-eicosane - D42, IS		94		1.031
70	1152-1148	69.088	1.058	biphenyl	154	5		1.059
71	1163-1158	69.658	1.067	†phenol, D5, IS + D0; 1:20	94	115	.44(ME)	1.068
72	1201-1197	71.628	1.096	a fatty acid (tentative)		14		1.098
75	1261-1258	74.751	1.143	similar to 3,3-dimethyl-1,5-di-t-butylbicyclo(3.1.0)hexan-2-one	230	13		
78	1408-1404	82.573	1.261	dimethyl terephthalate - D4, IS		94		
79	1512-1509	88.303	1.347	†diethylphthalate	222	46		
80	1672-1666	97.493	1.484	1-nitronaphthalene - D7, IS		40		1.496
81	1794-1791	104.608	1.591	†myristic acid	228	27	(1.08(ME))	

(continued)

TABLE D3. (continued)

Sequence[a]	Spectrum Number	RT	RRT	Compound Name[b]	MW	%IS[c]	Relative Retention Times[d]	
							2S1Q11	9S1Q11
82	1800–1798	104.960	1.596	†dibutylphthalate	278	457		
84	1931–1927	112.598	1.711	(†)pentadecanoic acid	242	12	(1.16(ME))	
86	2109–2102	122.985	1.867	†palmitic acid	256	46	(1.24(ME))	
87	2178–2173	127.006	1.927	(†)palmitoleic acid	254	17	(1.26(ME))	

a) The sequence number is used to label the peaks in the GC-MS chromatogram, Figure D3.

b) ME = methyl ester or methyl ether; IS = internal standard; † = a compound attributable to the 10-liter extraction blank.

c) Size (height) of the GC peak in the GC-MS chromatogram (see a, above) expressed as a percentage of the internal standard, hexaethylbenzene.

c) The values shown are the RRT values at which the compound was detected in the acid and neutral fraction, respectively.

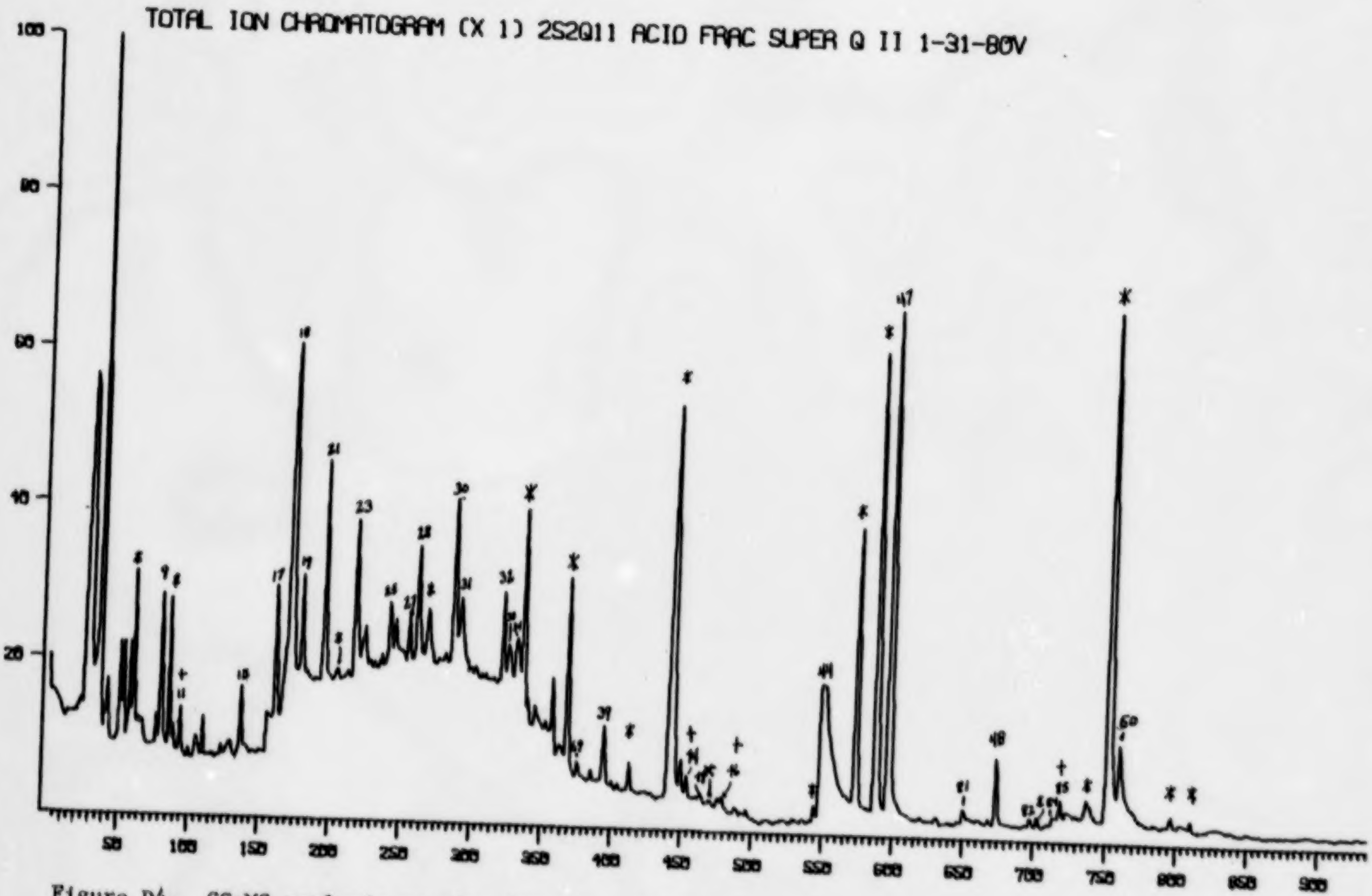

Figure D4. GC-MS analysis results for the acid fraction of the 10-liter reagent water sample, S2Q.

(continued)

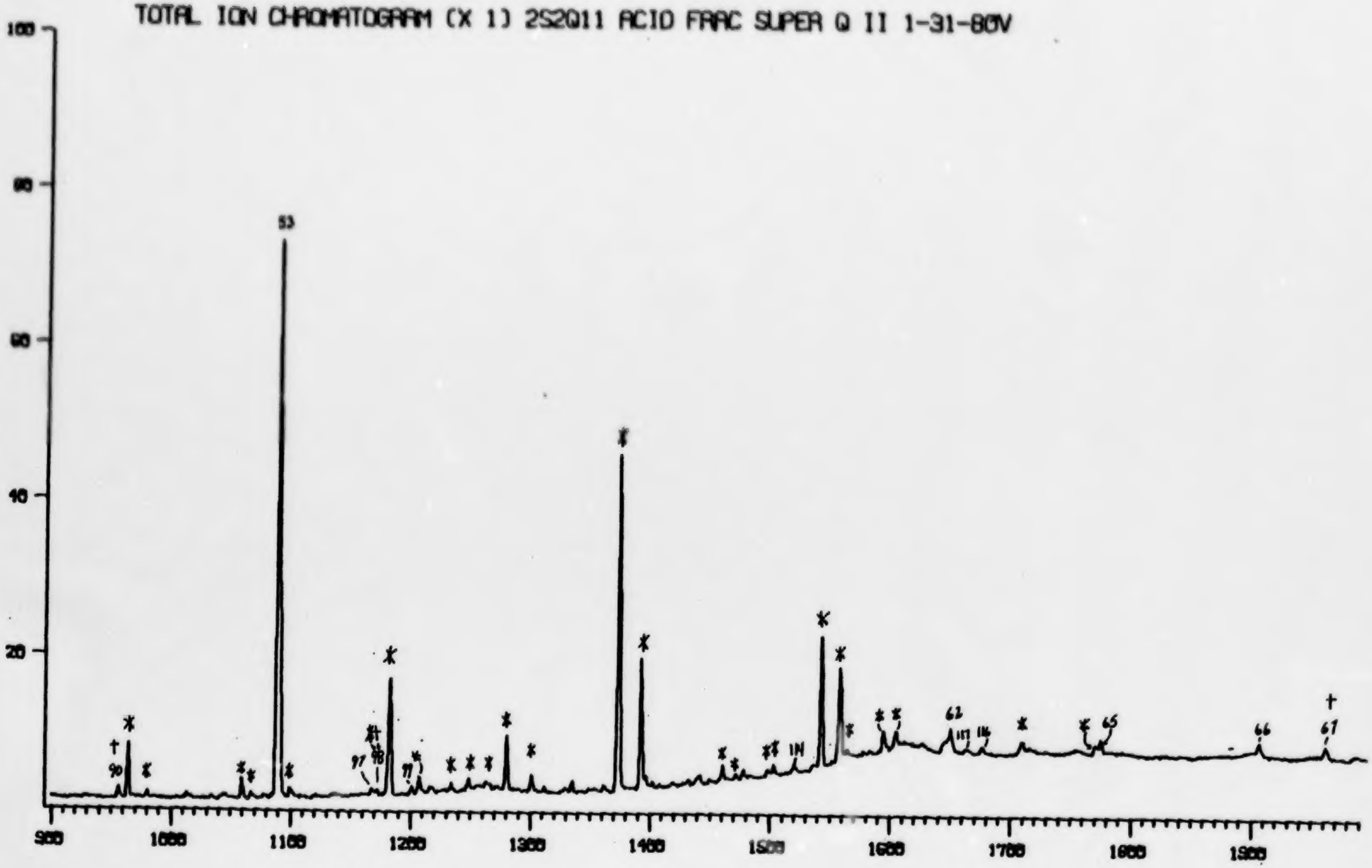

Figure D4. (Continued)

TABLE D4. GC-MS ANALYSIS RESULTS FOR THE ACID FRACTION OF THE 10-LITER REAGENT WATER SAMPLE, S2Q

Sequence[a]	Spectrum Number	RT	RRT	Compound Name[b]	Molecular Formula	Molecular Weight	GC Peak Size[c]		Match[d]	Proof[e]
							% IS	RS		
9	80-78	11.401	0.175	1-propanol	C3.H8.O1	60	27	3	918	B
11	94-92	12.178	0.187	†1,4-dioxane	C4.H8.O2	88	9	2	955	B
13	105-101	12.800	0.197	2-hexanone	C6.H12.O1	100	4	2	864	C
15	137-133	14.670	0.226	BP 45; m/e 71, 91, 114			14			
17	161-159	16.083	0.247	3-heptanone	C7.H14.O1	114	30	3	822	B
18	170-165	16.571	0.255	m/e 40, 48, 57, 75, 90						
19	179-176	17.056	0.262	BP 56; m/e 41, 42, 70						
21	194-192	17.856	0.275	BP 58; m/e 71, 85, 99, 114						
23	216-214	19.020	0.293	BP 40; m/e 47, 76, 58						
25	241-237	20.336	0.313	BP 59; m/e 70, 98						
27	255-252	21.071	0.324	BP 73; m/e 55, 41, 87, 88						
28	261-258	21.383	0.329	BP 59; m/e 72, 90, 41						
30	286-284	22.688	0.349	BP 55; m/e 41, 56, 70, 85, 98; similar to #31						
31	292-289	23.003	0.354	an alkane			28	3		
32	322-319	24.561	0.378	BP 55; m/e 73, 41						
33	326-324	24.771	0.381	an alkane			20	2		
34	332-329	25.088	0.386	an alkane			21	2		
39	395-391	28.375	0.437	BP 45; m/e 75, 87, 102, 132						
44	549-546	36.336	0.559	acetic acid (free acid, artifact)	C2.H4.O2	60	25	3	759	B
47	596-592	38.761	0.596	iso octanol	C8.H18.O1	130	91	4	964	B
48	673-669	42.756	0.658	1-octanol	C8.H18.O1	130	12	3	980	A
53	1091-1095	64.520	1.002	hexaethylbenzene, IS			100			
62	1650-1653	96.611	1.496	4,8,12-trimethyl-3,7,11-tridecatrienenitrile	C16.H15.N	231	5	2	937	C
65	1775-1780	104.245	1.613	n-alkane			3	1		
66	1901-1896	111.873	1.730	n-alkane			2	1		
67	1942-1935	114.363	1.769	†dihexyl adipate	C18.H34.O4	314	2	1	man	C
69	376-374	27.385	0.421	2-hydroxy propanoic acid, ME	C3.H6.O3	90	3	1	909	B
74	454-452	31.428	0.484	†octanoic acid, ME	C8.H16.O2	144	4	2	978	A
76	478-473	32.671	0.503	†2-butoxy ethanol	C6.H14.O2	118	3	1	962	A
77	464-467	31.948	0.492	a branched alkyl alcohol			2	1		
81	650-646	41.570	0.640	4-(acetyloxy)-2-butanone	C6.H10.O3	130	3	1	823	D
82	698-695	44.051	0.678	trimethyl phosphate, artifact	H3.O4.P	98	1	1	994	B
84	714-711	44.878	0.690	diethylene glycol monomethyl ether	C5.H12.O3	120	2	0	896	A

(continued)

TABLE D4. (continued)

Sequence[a]	Spectrum Number	RT	RRT	Compound Name[b]	Molecular Formula	Molecular Weight	GC Peak[c] Size % IS	GC Peak[c] Size RS	Match[d]	Proof[e]
85	719-716	45.138	0.694	†capric acid, ME	C10.H20.O2	172	5	1	man	A
90	955-953	57.346	0.882	†1-(2-butoxyethoxy)ethanol	C8.H18.O3	162	2	1	985	B
97	1167-1164	68.646	1.065	an alkane			1	1		
98	1171-1177	68.866	1.069	†phenol - D5, IS + D0, 1:3	C6.H6.O	94	1	0	921	A
99	1201-1197	70.518	1.094	an alkane aldehyde			2	1		
114	1520-1515	88.696	1.374	an alkane			2	1		
116	1676-1673	98.200	1.520	an alkane			1	1		
117	1663-1660	97.408	1.508	fatty acid, ME + alkene?			1	0		

a) The sequence number is used to label the peaks in the GC-MS chromatogram, Figure D4.

b) ME = methyl ester or methyl ether; IS = internal standard; † = a compound attributable to the 10-liter extraction blank.

c) Size (height) of the GC peak in the GC-MS chromatogram (see a, above) expressed as: %HEB, a percentage of the internal standard, hexaethylbenzene; RS, the relative size parameter explained in Section 5.

d) The quality index of the computer mass spectral library match (Finnigan INCOS software) where the value 1000 reflects a perfect fit of the data mass spectrum with the library mass spectrum.

e) Proof reflects the confidence level of the analyst: A, confirmed identification by comparison to data from a standard; B, highest confidence level for non-confirmable compounds; C, less than 80% confidence level; D, less than 50% confidence level.

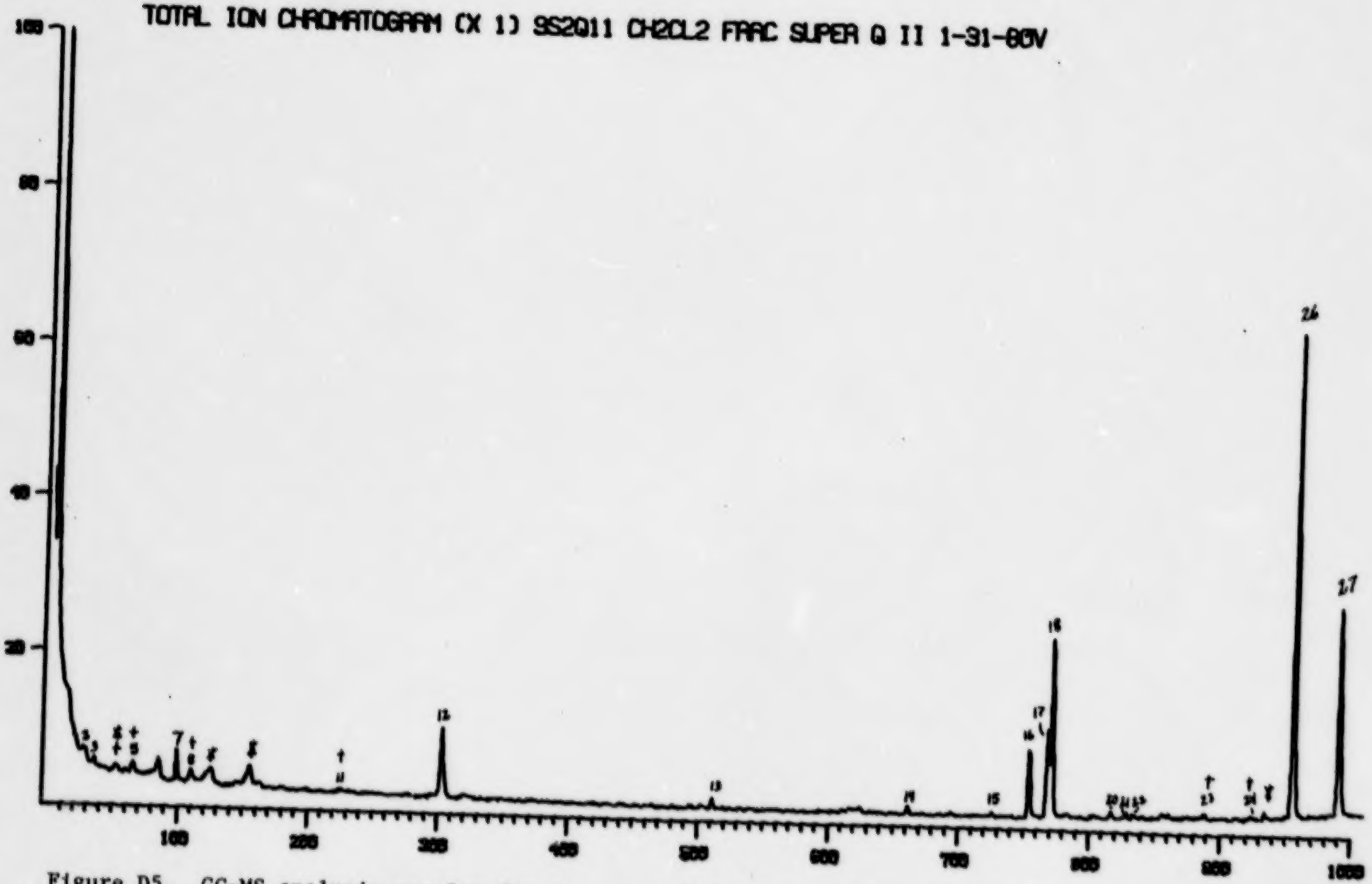

Figure D5. GC-MS analysis results for the aromatic/medium polarity fraction of the 10-liter reagent water sample, S2Q.

(continued)

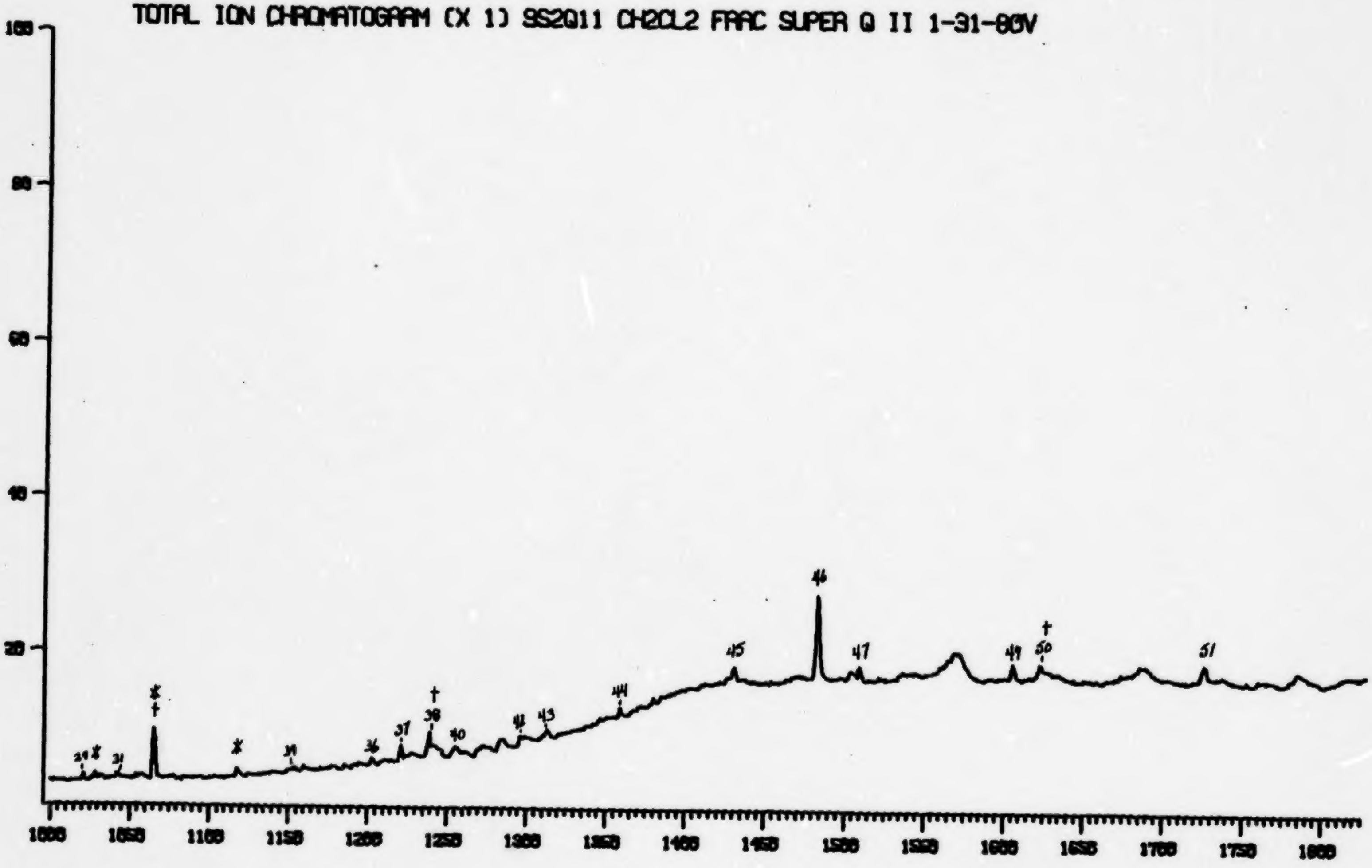

Figure D5. (Continued)

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TABLE D5. GC-MS ANALYSIS RESULTS FOR THE AROMATIC/MEDIUM POLARITY FRACTION OF THE 10-LITER REAGENT WATER SAMPLE, S2Q

Sequence[a]	Spectrum Number	RT	RRT	Compound Name[b]	Molecular Formula	Molecular Weight	GC Peak[c] Size % IS	RS	Match[d]	Proof[e]
2	29-33	7.448	0.115	2-hexanone	C6.H12.O1	100	3	1	955	B
3	36-33	7.976	0.123	an alkane			2	1		
5	65-62	10.156	0.156	†m-xylene	C8.H10	106	25	1	991	A
7	99-96	12.651	0.195	silicone compound			7	2		
8	110-106	13.450	0.207	†o-xylene	C8.H10	106	3	1	992	A
11	225-229	21.361	0.329	†1,2,4-trimethyl benzene	C9.H12	120	1	0	989	A
12	303-298	26.460	0.407	bromobenzene - D5, IS			14			
13	511-508	39.206	0.603	1,1,2,2-tetrachloroethane	C2.H2.CL4	166	25	1	976	A
14	662-658	47.841	0.736	1,2,4-trichlorobenzene	C6.H3.CL3	180	2	1	994	A
15	726-722	51.420	0.791	an alkane			1	0		
16	754-750	52.980	0.815	p-dibromobenzene - D4, IS			14			
17	768-764	53.773	0.827	nitrobenzene - D5, IS			18			
18	772-777	54.001	0.831	naphthalene - D8, IS, + D0; 7:1			37			
20	817-813	56.536	0.870	1,2,3,5-tetrachlorobenzene	C6.H2.CL4	214	2	1	973	A
21	829-824	57.221	0.880	1,2,4,5-tetrachlorobenzene	C6.H2.CL4	214	1	1	961	A
22	834-831	57.506	0.885	an alkane			1	0		
23	889-886	60.630	0.933	†2-methyl naphthalene	C11.H10	142	1	0	969	A
24	924-920	62.643	0.964	†1-methyl naphthalene	C11.H10	142	1	0	967	A
26	956-950	64.508	1.000	hexaethylbenzene, IS			100			
27	990-986	66.501	1.031	N-eicosane - D42, IS			43			
29	1021-1017	68.310	1.059	biphenyl	C12.H10	154	2	1	979	A
31	1042-1039	69.541	1.077	methyl myristate	C14.H28.O2	242	1	0	898	A
34	1154-1149	76.160	1.179	acenaphthalene	C12.H10	154	1	0	984	A
36	1203-1201	79.098	1.224	an alkane			2	1		
37	1221-1218	80.188	1.241	methyl palmitate	C17.H34.O2	270	35	1	937	A
38	1239-1234	81.286	1.258	†palmitic acid (tentative)	C16.H32.O2	256	6	2	900	D
40	1255-1252	82.261	1.273	dibenzofuran	C12.H8.O1	168	3	1	966	A
42	1297-1294	84.838	1.313	a silicone			2	1		
43	1313-1308	85.833	1.328	fluorene	C13.H10	166	2	1	947	A
44	1359-1357	88.713	1.372	an alkane			2	1		
45	1431-1428	93.278	1.443	an alkane			3	1		
46	1483-1479	96.590	1.494	1-nitronaphthalene - D7, IS			18			

(continued)

TABLE D5. (continued)

Sequence[a]	Spectrum Number	RT	RRT	Compound Name[b]	Molecular Formula	Molecular Weight	GC Peak[c] Size % IS	RS	Match[d]	Proof[e]
47	1510-1514	98.330	1.520	an alkane			3	1		
49	.1606-1602	104.485	1.615	an alkane			3	1		
50	1623-1619	105.575	1.632	†phenanthrene	C14.H10	178	3	1	984	A
51	1726-1719	112.190	1.734	an alkane			4	1		

a) The sequence number is used to label the peaks in the GC-MS chromatogram, Figure D5.

b) ME = methyl ester or methyl ether; IS = internal standard; † = a compound attributable to the 10-liter extraction blank.

c) Size (height) of the GC peak in the GC-MS chromatogram (see a, above) expressed as: %HEB, a percentage of the internal standard, hexaethyl benzene; RS, the relative size parameter explained in Section 5.

d) The quality index of the computer mass spectral library match (Finnigan INCOS software) where the value 1000 reflects a perfect fit of the data mass spectrum with the library mass spectrum.

e) Proof reflects the confidence level of the analyst: A, confirmed identification by comparison to data from a standard; B, highest confidence level for non-confirmable compounds; C, less than 80% confidence level; D, less than 50% confidence level.

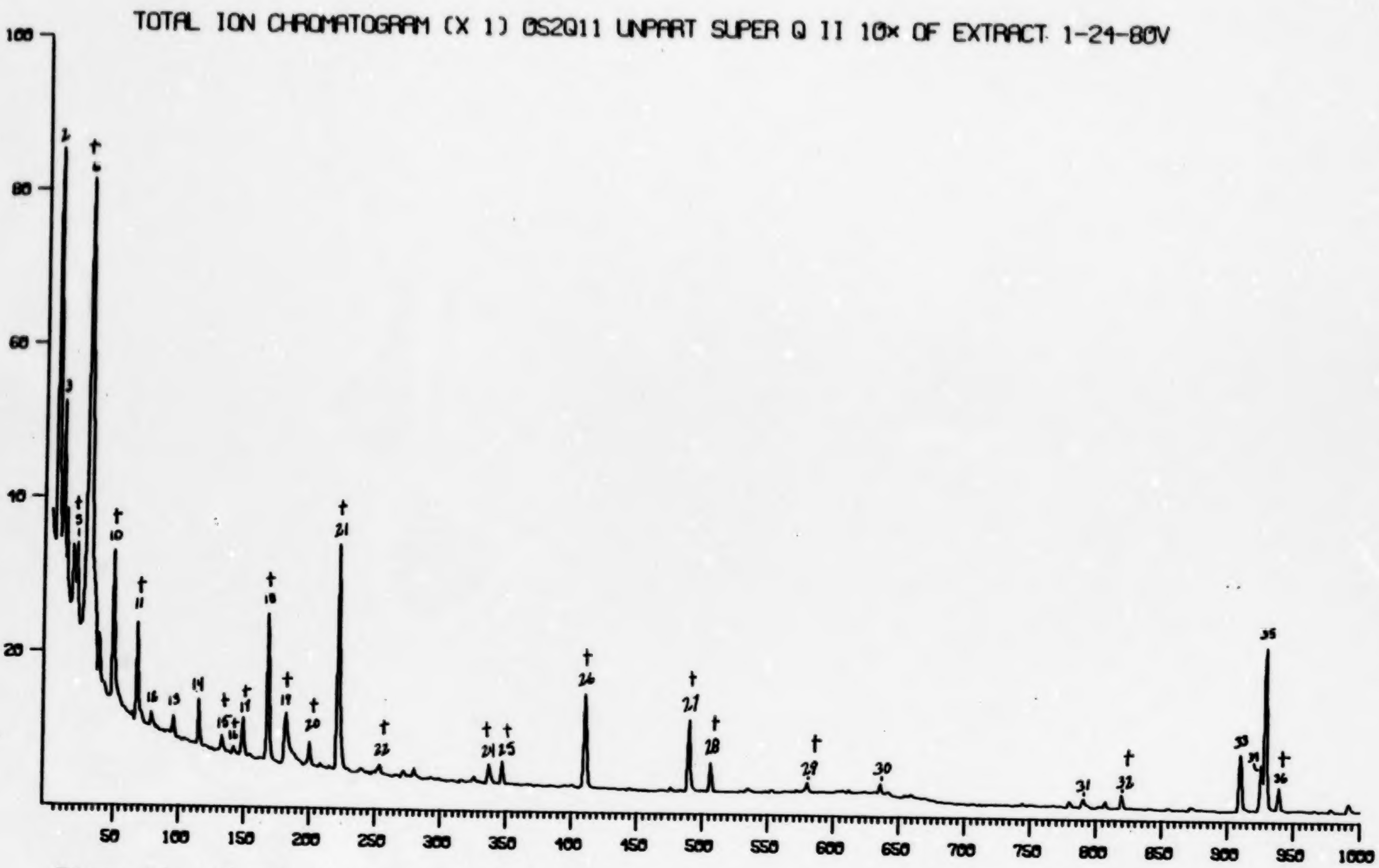

Figure D6. GC-MS analysis results for the unpartitioned aliquot of the 10-liter reagent water sample, S2Q.

(continued)

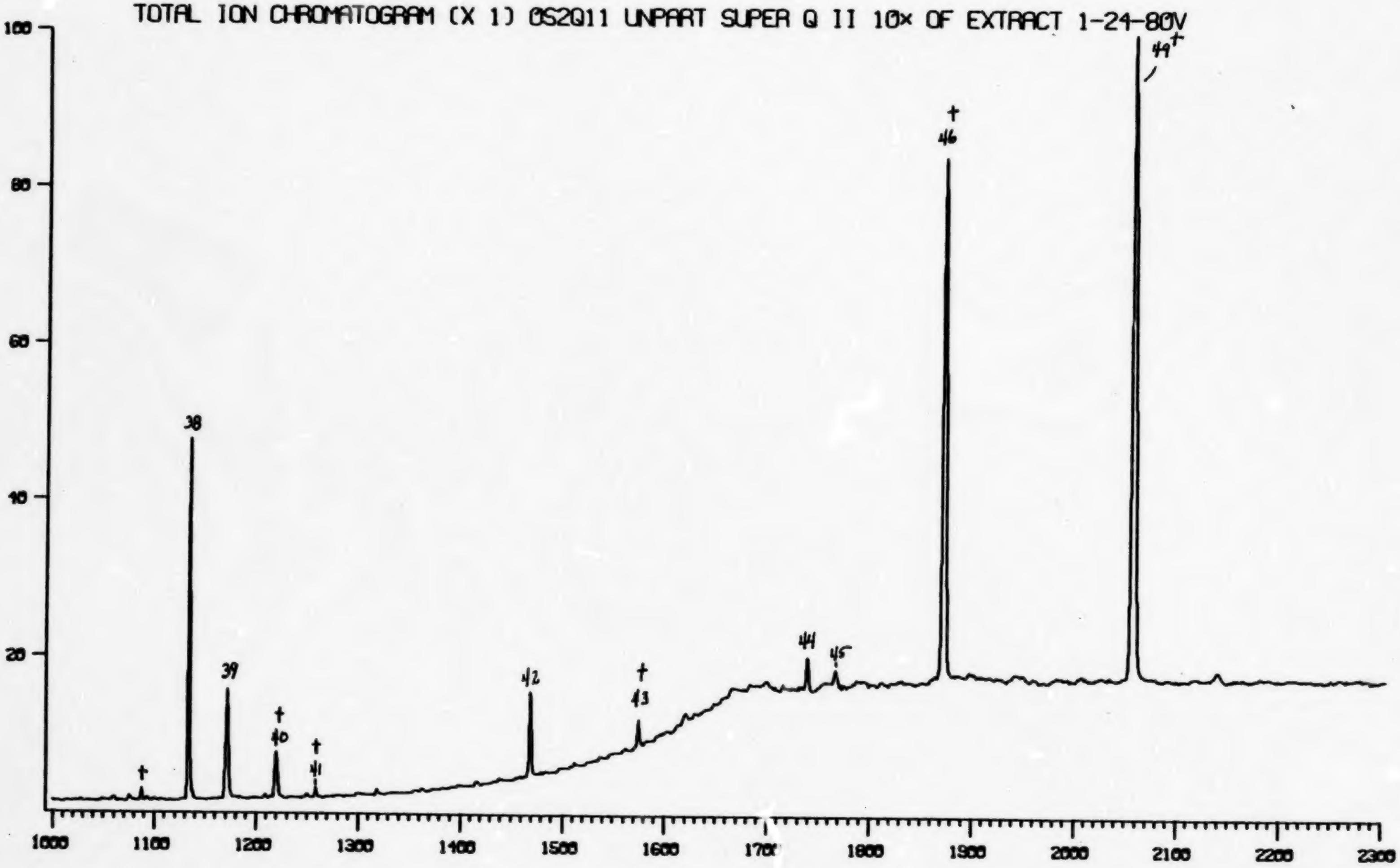

Figure D6. (Continued)

TABLE D6. GC-MS ANALYSIS RESULTS FOR THE UNPARTITIONED ALIQUOT OF THE 10-LITER REAGENT WATER SAMPLE, S2Q

Sequence[a]	Spectrum Number	RT	RRT	Compound Name[b]	MW	%IS[c]	Relative Retention Times[d] 2S2Q1	 9S2Q1
2	10-9	8.498	0.127	methyl butanoate	102	43		
3	13-12	8.665	0.130	trichloroethene plus ?	130	27		
5	21-24	9.103	0.137	†2-methyl propanenitrile	69	24		
6	27-23	9.426	0.141	†chloroform, solvent artifact	118	128		
10	49-45	10.588	0.159	†toluene	92	43		
11	68-65	11.583	0.174	†1,4-dioxane	88	28	.187	
12	79-77	12.153	0.182	butyl acetate	116	5		
13	96-92	13.036	0.196	an alkane		6		.123
14	115-113	14.025	0.210	decamethyl cyclopentasiloxane	370	13		
15	133-130	14.963	0.224	†ethyl benzene	106	5		(.142)
16	142-140	15.426	0.231	†p-xylene	106	2.5		.156
17	149-146	15.785	0.237	†m-xylene	106	11		
18	168-165	16.760	0.251	†BP 41; m/e 83, 97, 69, 54		41		.179
19	182-179	17.473	0.262	†cyclopentane carboxaldehyde	98	15		
20	200-196	18.390	0.276	†o-xylene	106	7		.207
21	222-218	19.508	0.293	†(chloromethyl)oxirane	92	64		
22	253-252	21.080	0.316	†3-chlorocyclohexene	116	3		
24	337-334	25.310	0.380	†cyclohexanone	98	6		
25	347-344	25.810	0.387	†2-ethoxy ethanol acetate	132	7		
26	411-407	29.015	0.435	†bromobenzene - D5, IS plus possible a tetrachloro propane	 180	27		.407
27	490-487	32.958	0.494	†2-butoxy ethanol	118	21	.503	
28	506-503	33.756	0.506	†chloroacetonitrile	75	9		
29	580-583	37.441	0.562	†2-cyclohexen-1-ol	98	3		
30	636-633	40.230	0.603	1,1,2,2-tetrachloroethane	166	3		.603
31	790-787	47.853	0.718	dihydro-2-furanone	86	2.5		
32	819-817	49.301	0.740	†4-chlorocyclohexanol	134	4		
33	910-906	53.821	0.807	p-dibromobenzene - D4, IS		16		.815
34	925-921	54.578	0.819	nitrobenzene - D5, IS		13		.827
35	929-926	54.785	0.822	naphthalene - D8, IS, + D0; 10:1		46		.831
36	939-935	55.296	0.829	†1,3-dichloro-2-propanol	128	7		
38	1134-1129	65.128	1.000	hexaethylbenzene, IS				
39	1171-1165	67.033	1.029	N-eicosane - D42, IS		31		1.031

(continued)

TABLE D6. (continued)

Sequence[a]	Spectrum Number	RT	RRT	Compound Name[b]	MW	%IS[c]	Relative Retention Times[d]	
							2S2Q1	9S2Q1
40	1219-1216	69.496	1.066	†phenol - D5, IS + D0; 1:3	94	13	1.069	
41	1258-1256	71.496	1.096	†myristic acid ?; fatty acid	228	3	(1.078)	1.099
42	1468-1463	82.415	1.259	dimethyl terephthalate - D4, IS	198	24		
43	1575-1571	88.183	1.346	†diethyl phthalate	222	8	1.354	
44	1739-1736	97.373	1.484	1-nitronaphthalene - D7, IS		9		1.494
45	1767-1761	98.970	1.508	3-hexyl tetrahydro-6,6,9-trimethyl dibenzopyran-1-ol	328	5		
46	1870-1867	104.785	1.595	†di-n-butyl phthalate	278	146	1.609	
49	2055-2051	115.263	1.752	†dihexyl adipate	314	179	1.769	

a) The sequence number is used to label the peaks in the GC-MS chromatogram, Figure D6.

b) ME = methyl ester or methyl ether; IS = internal standard; † = a compound attributable to the 10-liter extraction blank.

c) Size (height) of the GC peak in the GC-MS chromatogram (see a, above) expressed as a percentage of the internal standard, hexaethylbenzene.

d) The values shown are the RRT values at which the compound was detected in the acid and neutral fraction, respectively.

APPENDIX E

ANALYSIS RESULTS FOR CINCINNATI TAP WATER AND LYOPHILIZED CINCINNATI TAP WATER

Appendix E contains labeled GC-MS chromatograms for analysis of the unpartitioned aliquot, acid fraction and neutral fraction for the Cincinnati tap water and lyophilized Cincinnati tap water samples. Each chromatogram is accompanied by a table immediately following it in which, for each labeled peak in the chromatogram, the mass spectral data interpretation results are given.

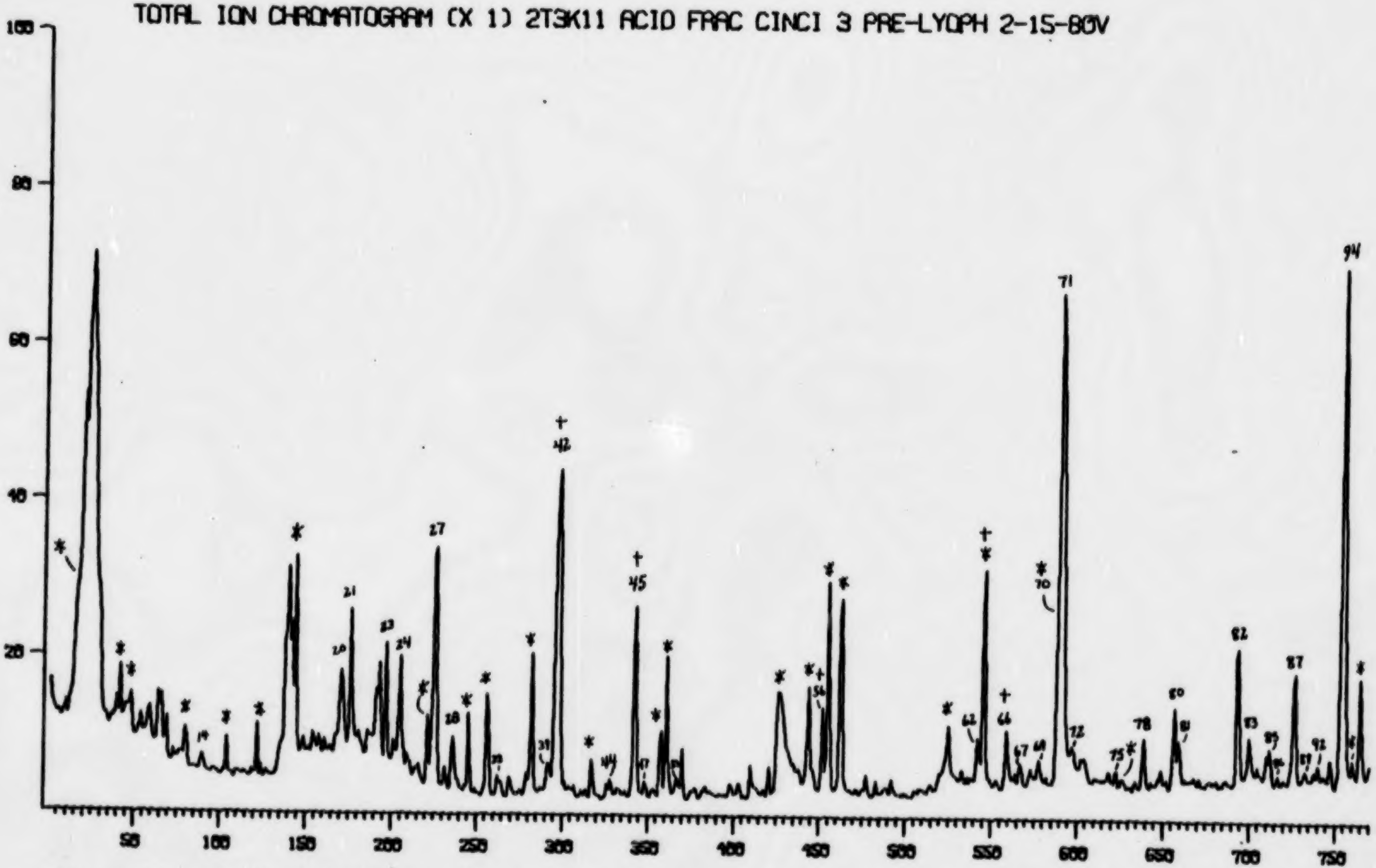

Figure E1. GC-MS analysis results for the acid fraction of the 10-liter Cincinnati tap water sample, T3K.

(continued)

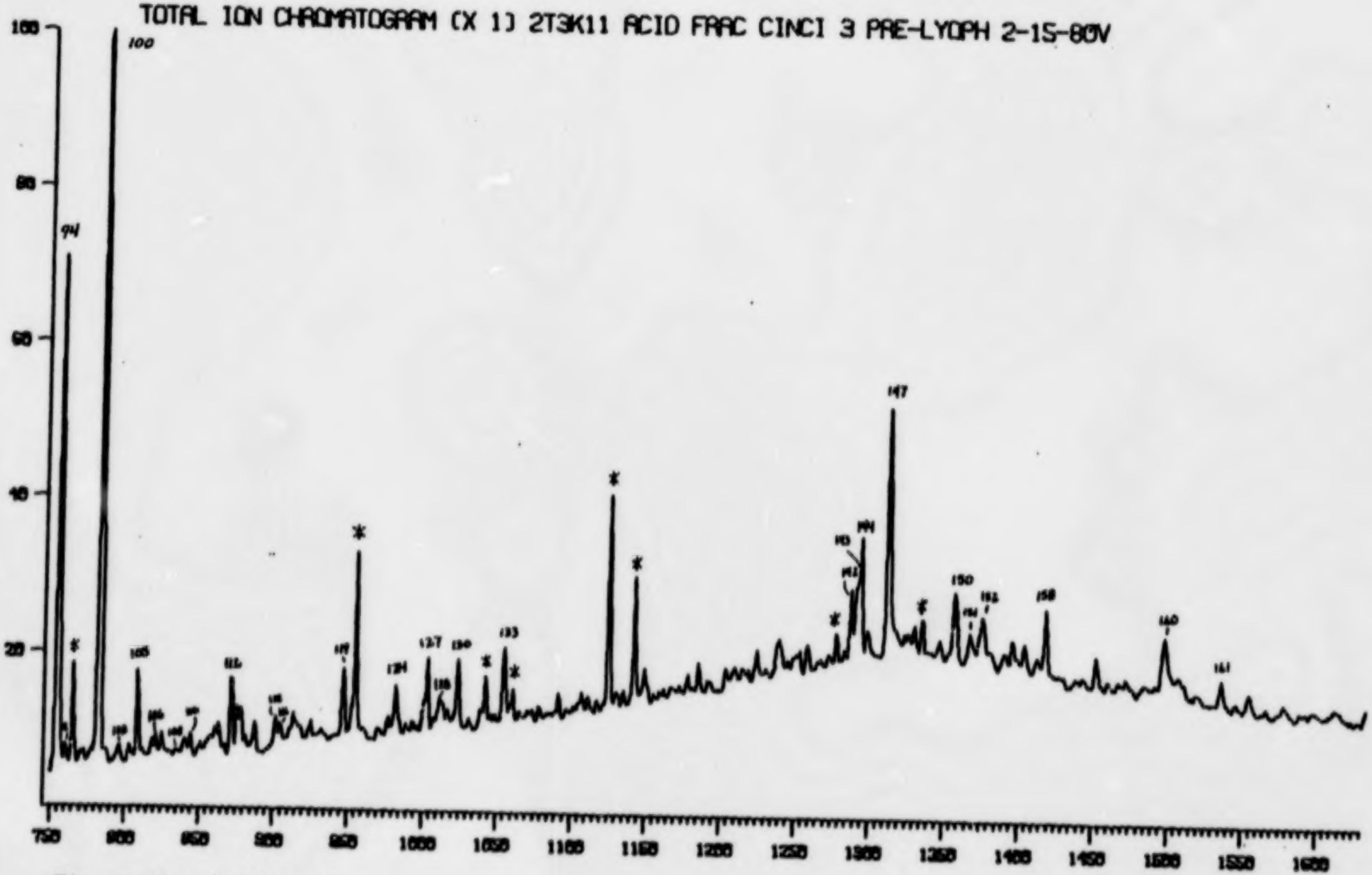
TOTAL ION CHROMATOGRAM (X 1) 2T3K11 ACID FRAC CINCI 3 PRE-LYOPH 2-15-80V

Figure E1. (Continued)

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TABLE E1. GC-MS ANALYSIS RESULTS FOR THE ACID FRACTION OF THE 10-LITER CINCINNATI TAP WATER SAMPLE, T[illegible]

Sequence[a]	Spectrum Number	RT	RRT	Compound Name[b]	Molecular Formula	Molecular Weight	GC Peak[c] Size % IS	RS	Match[d]	Proof[e]
14	90-86	12.486	0.192	1-methoxy-2-methyl-2-propanol, probable artifact	C5.H12.O2	104	5	2	950	C
20	171-166	18.780	0.289	3-hexanol	C6.H14.O1	102	7	2	956	B
21	176-173	19.133	0.294	BP 40 or 46; m/e 58, 76, 88 (101)						
23	197-194	20.598	0.317	BP 74; m/e 87, 103						
24	205-203	21.155	0.325	2-ethylhexanoic acid, ME	C8.H16.O2	144	34	4	972	A
27	227-231	22.680	0.349	3-methoxy-3-methyl-2-butanone	C6.H12.O2	116	67	4	899	C
28	236-233	23.306	0.359	heptanoic acid, ME	C7.H14.O2	130	15	3	993	A
33	264-260	25.226	0.388	a C-6 alcohol			6			
39	291-287	27.045	0.416	2-hydroxy propanoic acid, ME	C3.H6.O3	90	9	2	909	B
42	297-293	27.446	0.422	†phenol, ME-D5, IS + DO (sat.); ratio less than 1:10	C6.H6.O1	94	90		824	A
44	328-324	29.505	0.454	dichloro acetic acid, ME	C2.H2.O2.CL2	128	6	2	956	A
45	342-339	30.431	0.468	†octanoic acid, ME	C8.H16.O2	144	54	4	890	A
47	348-346	30.826	0.474	2-chloroethanol	C2.H5.O1.CL1	80	5	2	860	C
53	367-364	32.076	0.493	o-cresol, ME + ?	C7.H8.O1	108	6	2	935	B
56	452-449	37.583	0.578	†nonanoic acid, ME	C9.H18.O2	158	26	3	980	A
62	542-539	43.338	0.667	levulinic acid, ME + MW 138	C5.H8.O3	116	17	3	921	A
66	559-556	44.405	0.683	†capric acid, ME	C10.H20.O2	172	18	3		A
67	567-570	44.910	0.691	succinic acid, di-ME	C4.H6.O4	118	8	2	865	A
69	578-575	45.598	0.702	mixture? 4-methyl-4-nitropentanoic acid, ME	C6.H11.O4.N	161	9	2	827	C
70	588-585	46.226	0.711	benzoic acid, ME - D5, IS						
71	590-584	46.351	0.713	benzoic acid, ME (saturated ions)	C7.H6.O2	122	138	5	805	A
72	597-599	46.796	0.720	(chloromethyl)methyl mercury	C2.H5.CL.HG	266	12	3	man	C
75	623-620	48.451	0.745	an ethylene glycol ether			5	2		
78	639-636	49.456	0.761	BP 101; m/e 55, 73, 109, 125, 140			19	3		
80	657-654	50.585	0.778	BP 69; m/e 56, 115, 87, 99, 131			23	3		
81	659-661	50.710	0.780	o-toluic acid, ME + m/e 84, 69, 65	C8.H8.O2	136	14	3	980	A
82	693-691	52.828	0.813	similar to (methylisopropylcyclohexyl)acetate			30	3		
83	700-697	53.261	0.819	m-toluic acid, ME	C8.H8.O2	136	15	3	948	A
85	712-715	54.001	0.831	p-toluic acid, ME	C8.H8.O2	136	11	3	859	A
86	717-715	54.311	0.836	an unsaturated fatty acid, ME			4			
87	727-722	54.930	0.845	phenylacetic acid, ME	C8.H8.O2	136	32	3	865	A
89	733-729	55.303	0.851	2,6-dimethylbenzoic acid, ME	C9.H10.O2	150	4	3	957	A
92	740-736	55.735	0.857	salicyclic acid, ME	C7.H6.O3	138	6	3	987	A
94	755-750	56.661	0.872	2,3-dimethyl maleic acid, di-ME +	C6.H8.O4	144	145	5	man	A
				ethosuximide, N-methyl derivative	C7.H11.N.O2	141			man	A

(continued)

TABLE E1. (continued)

Sequence[a]	Spectrum Number	RT	RRT	Compound Name[b]	Molecular Formula	Molecular Weight	GC Peak[c] Size % IS	GC Peak[c] Size RS	Match[d]	Proof[e]
100	782-778	58.316	0.897	2-ethyl-3-methyl maleic acid, di-ME	C7.H10.O4	158	208	5	963	B
103	796-790	59.173	0.910	m-chlorobenzoic acid, ME	C7.H5.O2.CL	156	6	2	922	A
105	808-805	59.913	0.922	hydrocinnamic acid, ME	C9.H10.O2	150	27	3	994	A
106	821-815	60.715	0.934	3-hydroxynonanoic acid, ME	C9.H18.O3	174	7	2	man	C
108	835-832	61.575	0.947	benzyl alcohol plus ?	C7.H8.O1	108	2	1	946	A
110	844-842	62.131	0.956	2,4,6-trimethyl benzoic acid, ME	C10.H12.O2	164	7	2	925	A
112	871-868	63.808	1.000	hexaethylbenzene, IS			23			
115	902-898	65.736	1.030	MW 192; BP 177; m/e 192, 161, 149			16	3		
116	904-908	65.865	1.032	an organo mercury compound			9	2		
119	947-943	68.671	1.075	phenol (free acid); D5 + D0; 1:25	C6.H6.O1	94	21	3	997	A
124	982-978	70.860	1.109	phenoxy acetic acid, ME	C8.H8.O3	152	15	3	997	A
127	1003-1005	72.176	1.129	2-methoxybenzoic acid, ME	C8.H8.O3	152	22	3	941	A
128	1011-1008	72.678	1.136	3,5-dimethyl phenol, mixture	C8.H10.O1	122	9	2	920	C
130	1023-1019	73.436	1.148	4-methoxy benzoic acid, ME (anisic acid, ME)	C8.H8.O3	152	20	3	977	A
133	1055-1053	75.473	1.179	clofibric acid, ME	C10.H11.O3.CL	214	21	3	997	A
142	1287-1285	90.436	1.410	a fatty dienoic acid, ME			21			
143	1290-1288	90.633	1.413	3,4-dimethoxy benzoic acid, ME	C9.H10.O4	182	36	4	989	B
144	1294-1296	90.898	1.417	α,4-dihydroxy-3-methoxy phenyl acetic acid, ME	C9.H10.O5	198	36	4	744	C
147	1312-1308	92.081	1.435	BP 151; m/e 165, 180, 194; mixture MW 180 and 194			72	4		
150	1357-1353	95.055	1.481	BP 151; m/e 208, 198			23	3		
151	1367-1363	95.718	1.491	a 3-hydroxy fatty acid, ME			10	3		
152	1376-1371	96.318	1.500	mixture, including a 2-methyl fatty acid, ME			19	3		
158	1418-1414	99.140	1.544	similar to (isopropylphenoxy)methanol acetate			21	3		
160	1498-1493	104.526	1.626	BP 43; m/e 55, 203, 218, 221			19	3		
161	1535-1532	107.028	1.665	4-(1,5-dimethyl-3-oxohexyl)-1-cyclohexene carboxylic acid, ME	C15.H24.O3	252	10	3	975	B

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a) The sequence number is used to label the peaks in the GC-MS chromatogram, Figure E1.

b) ME = methyl ester or methyl ether; IS = internal standard; † = a compound attributable to the 10-liter extraction blank.

c) Size (height) of the GC peak in the GC-MS chromatogram (see a, above) expressed as: %HEB, a percentage of the internal standard, hexaethyl benzene; RS, the relative size parameter explained in Section 5.

d) The quality index of the computer mass spectral library match (Finnigan INCOS software) where the value 1000 reflects a perfect fit of the data mass spectrum with the library mass spectrum.

e) Proof reflects the confidence level of the analyst: A, confirmed identification by comparison to data from a standard; B, highest confidence level for non-confirmable compounds; C, less than 80% confidence level; D, less than 50% confidence level.

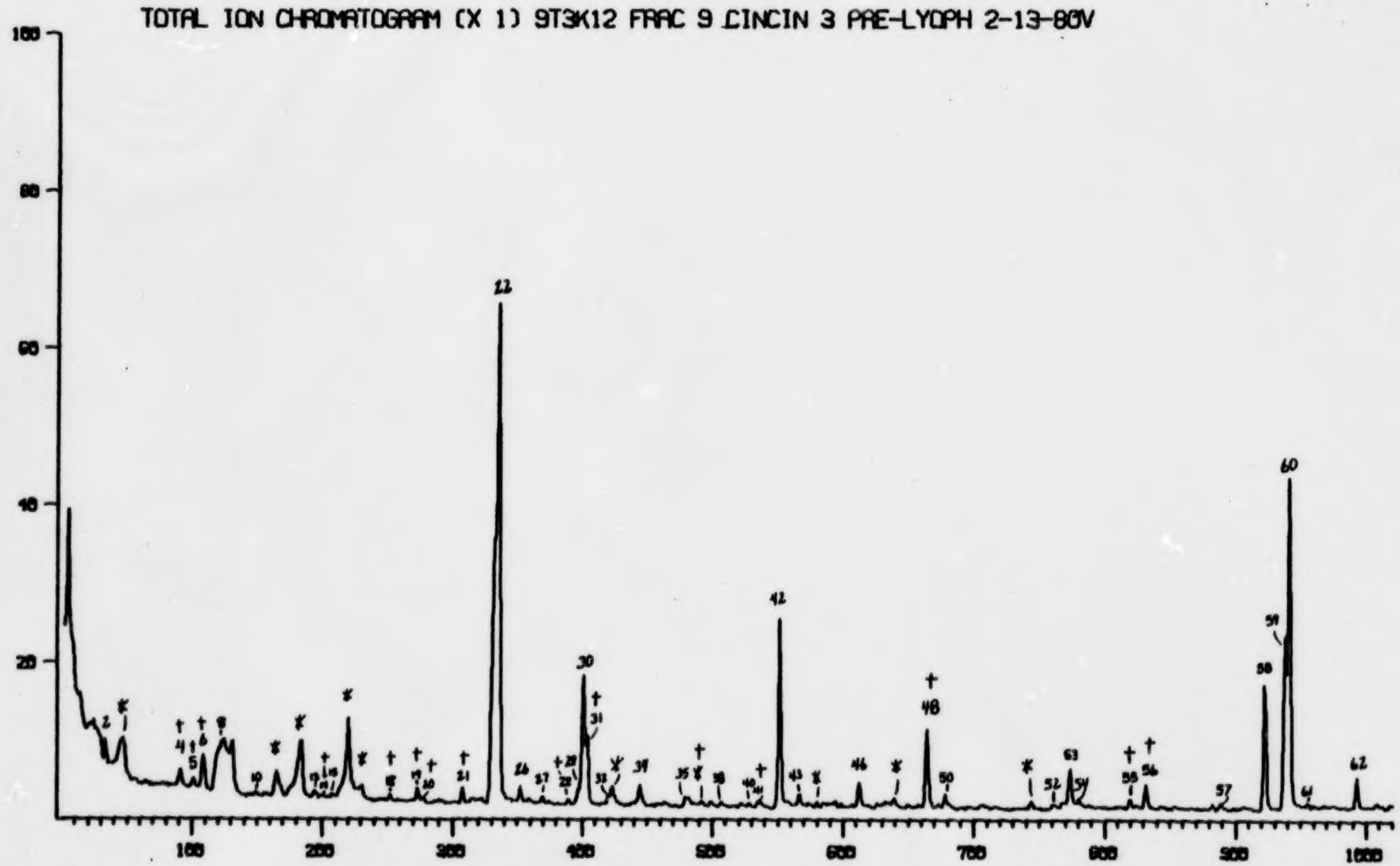

Figure E2. GC-MS analysis results for the aromatic/medium polarity fraction of the 10-liter Cincinnati tap water sample, T3K.

(continued)

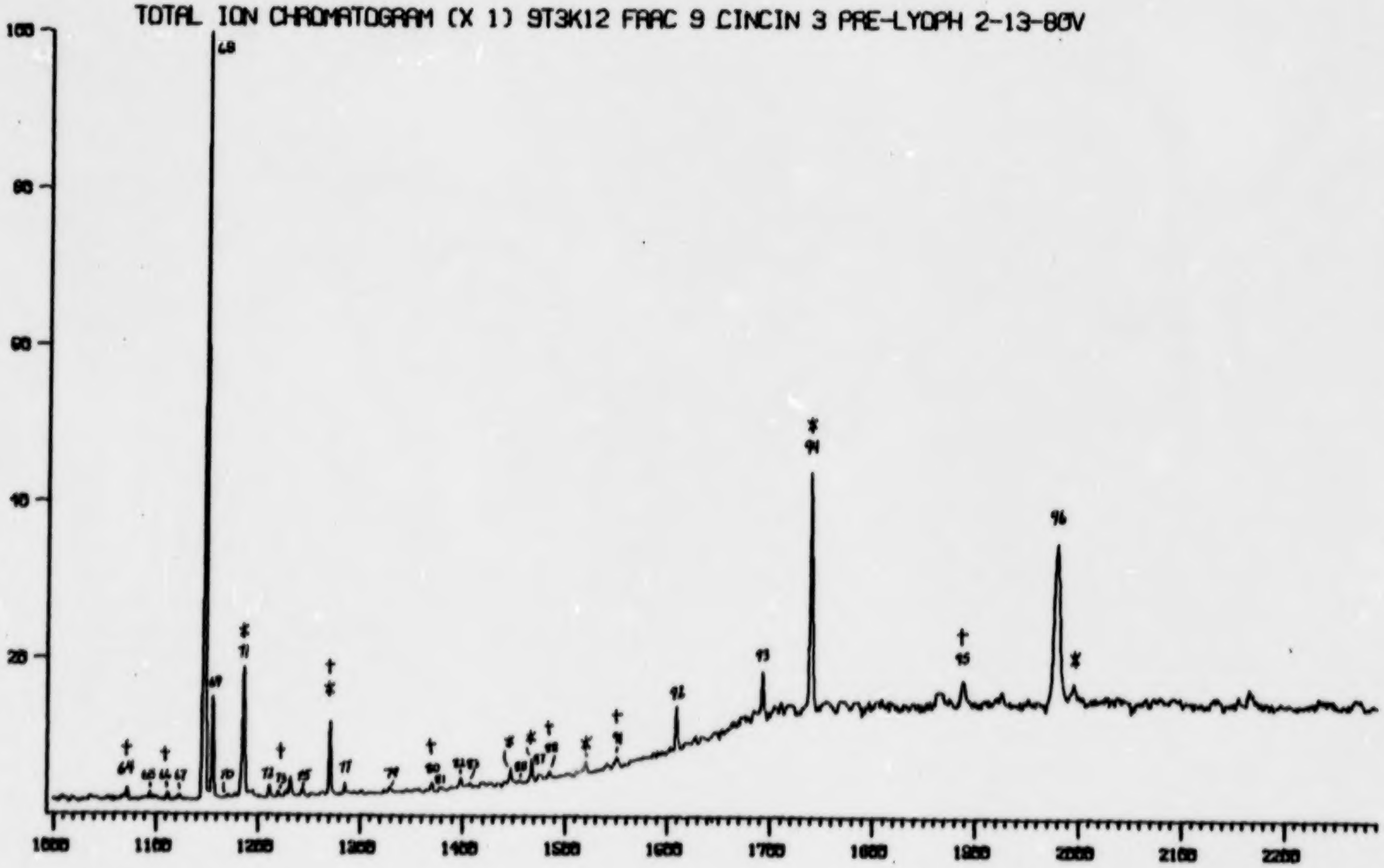

Figure E2. (Continued)

TABLE E2. GC-MS ANALYSIS RESULTS FOR THE AROMATIC/MEDIUM POLARITY FRACTION OF THE 10-LITER CINCINNATI TAP WATER SAMPLE, T3K

Sequence[a]	Spectrum Number	RT	RRT	Compound Name[b]	Molecular Formula	Molecular Weight	GC Peak[c] Size		Match[d]	Proof[e]
							% IS	RS		
2	33-31	7.443	0.115	2-butyl THF	C8.H16.O	128	03	1	958	C
4	91-87	10.535	0.162	†ethylbenzene	C8.H10	106	02	1	997	A
5	101-98	11.058	0.170	†p-xylene	C8.H10	106	01	0	994	A
6	108-105	11.423	0.176	†m-xylene	C8.H10	106	04	2	996	A
8	122-114	12.160	0.187	bromodichloro methane	C.H.CL2.BR	162	07	2	962	A
10	149-146	13.565	0.209	weak; 2,6-dimethyl-4-heptanone	C9.H18.O1	142	005	0	879	C
13	194-191	15.886	0.244	4-methylene-1-isopropyl cyclohexene	C10.H16	136	01	0	978	C
14	199-197	16.143	0.248	†propylbenzene	C9.H12	120	01	0	933	A
15	207-203	16.555	0.255	chlorobenzene, weak	C6.H5.CL	112	005	0	953	A
18	252-248	18.853	0.290	†1,3,5-trimethylbenzene	C9.H12	120	01	0	988	A
19	273-270	19.923	0.307	†styrene	C8.H8	104	015	1	992	A
20	277-282	20.126	0.310	†o-ethyl toluene	C9.H12	120	005	0	960	A
21	308-303	21.700	0.334	†1,2,4-trimethyl benzene	C9.H12	120	02	1	993	A
22	335-340	23.080	0.355	dibromochloro methane	C.H.CL.BR2	206	65	4	946	A
26	352-348	23.951	0.368	3-bromohexane	C6.H13.BR	164	02	1	966	D
27	369-366	24.808	0.382	5-methyl-2-hexanol	C7.H16.O1	116	01	0	945	C
28	390-387	25.870	0.398	†1,2,3-trimethyl benzene	C9.H12	120	01	0	985	A
29	397-393	26.221	0.403	bromobenzene - D5, IS plus						
				2-methylcyclopentanol	C6.H12.O1	100	4	2	869	A
30	401-396	26.426	0.407	bromobenzene - D5, IS						
31	404-408	26.583	0.409	†1,1,1,3-tetrachloropropane	C3.H4.CL4	180	09	1	man	C
32	420-417	27.393	0.421	(1-methylbutyl)oxirane	C7.H14.O1	114	015	0	942	B
34	444-440	28.600	0.440	1-(dichloromethyl)naphthalene	C11.H8.CL2	210	03	1	man	B
35	480-477	30.403	0.468	nonanal	C9.H18.O1	142	015	0	917	A
38	507-504	31.761	0.489	m-dichlorobenzene	C6.H4.CL2	146	01	0	972	A
40	528-525	32.815	0.505	hexachloroethane	C2.CL6	234	01	0	896	A
41	535-531	33.165	0.510	†2-cyclohexen-1-one	C6.H8.O1	96	01	0	988	A
42	551-544	33.966	0.523	bromoform plus	C.H.BR3	250	21	3	957	A
				p-dichlorobenzene	C6.H4.CL2	146	4	2	man	A
43	567-563	34.778	0.535	chlorinated, weak			015	1		
46	612-617	37.020	0.570	o-dichlorobenzene	C6.H4.CL2	146	03	1	999	A
48	664-658	39.621	0.610	†benzaldehyde	C7.H6.O1	106	02	2	999	A
50	678-676	40.320	0.620	(2-chloroethyl)ether	C4.H8.O.CL2	142	02	1	987	A

(continued)

TABLE E2. (continued)

Sequence[a]	Spectrum Number	RT	RRT	Compound Name[b]	Molecular Formula	Molecular Weight	GC Peak[c] Size		Match[d]	Proof[e]
							% IS	RS		
52	761-757	44.443	0.684	a branched alkane			01	0		
53	773-771	45.040	0.693	benzonitrile	C7.H5.N	103	05	2	999	A
54	780-778	45.391	0.698	a silicone			01	0		
55	819-816	47.330	0.728	†1,2,4-trichlorobenzene	C6.H3.CL3	180	015	0	987	A
56	832-828	47.983	0.738	†4-chlorocyclohexanol	C6.H11.O.CL	134	03	1	881	C
57	888-885	50.771	0.781	an alkane			01	0		
58	922-918	52.466	0.807	p-dibromobenzene - D4, IS						
59	938-933	53.280	0.820	nitrobenzene - D5, IS + D0; 3:1	C6.H5.N.O2	123	05	2	man	A
60	941-946	53.436	0.822	naphthalene-D8, IS + D0; 7:1	C10.H8	128	01	1	man	A
61	955-952	54.150	0.833	m-dimethoxybenzene	C8.H10.O2	138	01	0	974	B
62	993-989	56.065	0.863	1-methyl-2-nitrobenzene	C7.H7.O2.N	137	04	2	978	B
64	1072-1069	60.050	0.924	†2-methyl naphthalene	C11.H10	142	015	1	987	A
65	1094-1090	61.166	0.941	1-methyl-4-nitrobenzene	C7.H7.O2.N	137	01	0	954	B
66	1112-1109	62.080	0.955	†1-methyl naphthalene	C11.H10	142	01	0	985	A
67	1123-1119	62.635	0.964	an alkane			01	0		
68	1148-1142	63.930	1.000	hexaethylbenzene, IS			100			
69	1155-1152	64.306	1.006	benzylcyanide	C8.H7.N	117	14	3	998	A
70	1171-1167	65.130	1.018	2-chloroaniline	C6.H6.N.CL	127	005	0	935	A
71	1186-1180	65.910	1.030	N-eicosane - D42, IS						
72	1211-1207	67.210	1.050	N-cyclohexylidene methanamine	C7.H13.N	111	02	1	865	D
73	1220-1217	67.676	1.058	†biphenyl	C12.H10	154	01	0	984	A
75	1244-1238	68.928	1.077	methyl myristate (artifact) plus	C15.H30.O2	242	01	0	833	A
				phenyl ether	C12.H10.O1	170		0	man	A
77	1285-1281	71.066	1.110	a poly chlorinated alkane (hexachloro pentane?)	C5.H6.CL6	276	02	1	man	D
79	1329-1326	73.366	1.145	an alkane			01	0		
80	1370-1366	75.525	1.178	†acenaphthene	C12.H10	154	01	0	992	A
81	1378-1374	75.946	1.185	1,4,6-trimethyl naphthalene	C13.H14	170	01	0	783	A
82	1398-1393	77.001	1.201	7,11-dimethyl-3-methyl-1,6,10-dodecatriene	C15.H24	204	015	0	941	C
83	1407-1410	77.480	1.208	1-methyl barbital plus	C9.H14.O3.N2	198	0.2	0	736	B
				pentylbenzoate	C12.H16.O2	192	0.2	0	827	C
85	1456-1454	80.106	1.249	4-bromo-2-methoxy-5-methyl phenol (weak)	C8.H9.O2.BR	216	005	0	665	C
87	1475-1471	81.126	1.265	weak (dimethyl diphenyl) methane	C15.H16	196	01	0	man	B
88	1485-1482	81.666	1.273	†dibenzofuran	C12.H8.O1	168	015	0	995	A
91	1550-1544	85.188	1.327	†fluorene	C13.H10	166	02	1	963	A

(continued)

TABLE E2. (continued)

Sequence[a]	Spectrum Number	RT	RRT	Compound Name[b]	Molecular Formula	Molecular Weight	GC Peak[c] Size % IS	RS	Match[d]	Proof[e]
92	1609-1606	88.438	1.377	2,6-dinitrotoluene	C7.H6.O4.N2	182	06	2	969	A
93	1692-1690	93.118	1.449	2,4-dinitrotoluene	C7.H6.O4.N2	182	065	2	991	A
94	1739-1735	95.825	1.491	1-nitronaphthalene - D7, IS						
95	1887-1884	104.313	1.621	†phenanthrene	C14.H10	178	035	1	985	A
96	1979-1969	109.565	1.702	4,8,12-trimethyl-3,7,11-tridecatriene nitrile	C16.H25.N	231	22	3	941	D

a) The sequence number is used to label the peaks in the GC-MS chromatogram, Figure E2.

b) ME = methyl ester or methyl ether; IS = internal standard; † = a compound attributable to the 10-liter extraction blank.

c) Size (height) of the GC peak in the GC-MS chromatogram (see a, above) expressed as: %HEB, a percentage of the internal standard, hexaethyl benzene; RS, the relative size parameter explained in Section 5.

d) The quality index of the computer mass spectral library match (Finnigan INCOS software) where the value 1000 reflects a perfect fit of the data mass spectrum with the library mass spectrum.

e) Proof reflects the confidence level of the analyst: A, confirmed identification by comparison to data from a standard; B, highest confidence level for non-confirmable compounds; C, less than 80% confidence level; D, less than 50% confidence level.

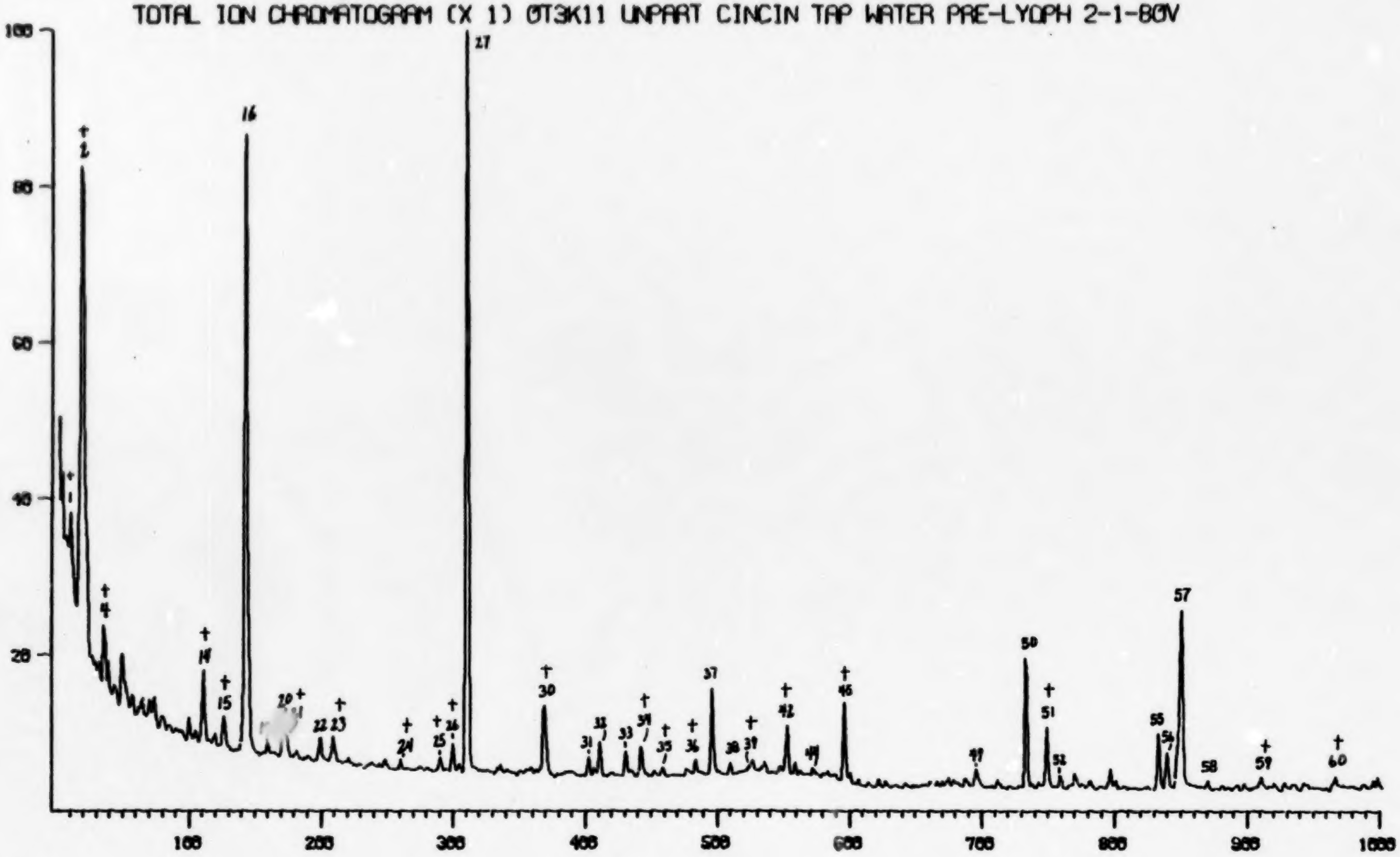

Figure E3. GC-MS analysis results for the unpartitioned aliquot of the 10-liter Cincinnati tap water sample, T3K.

(continued)

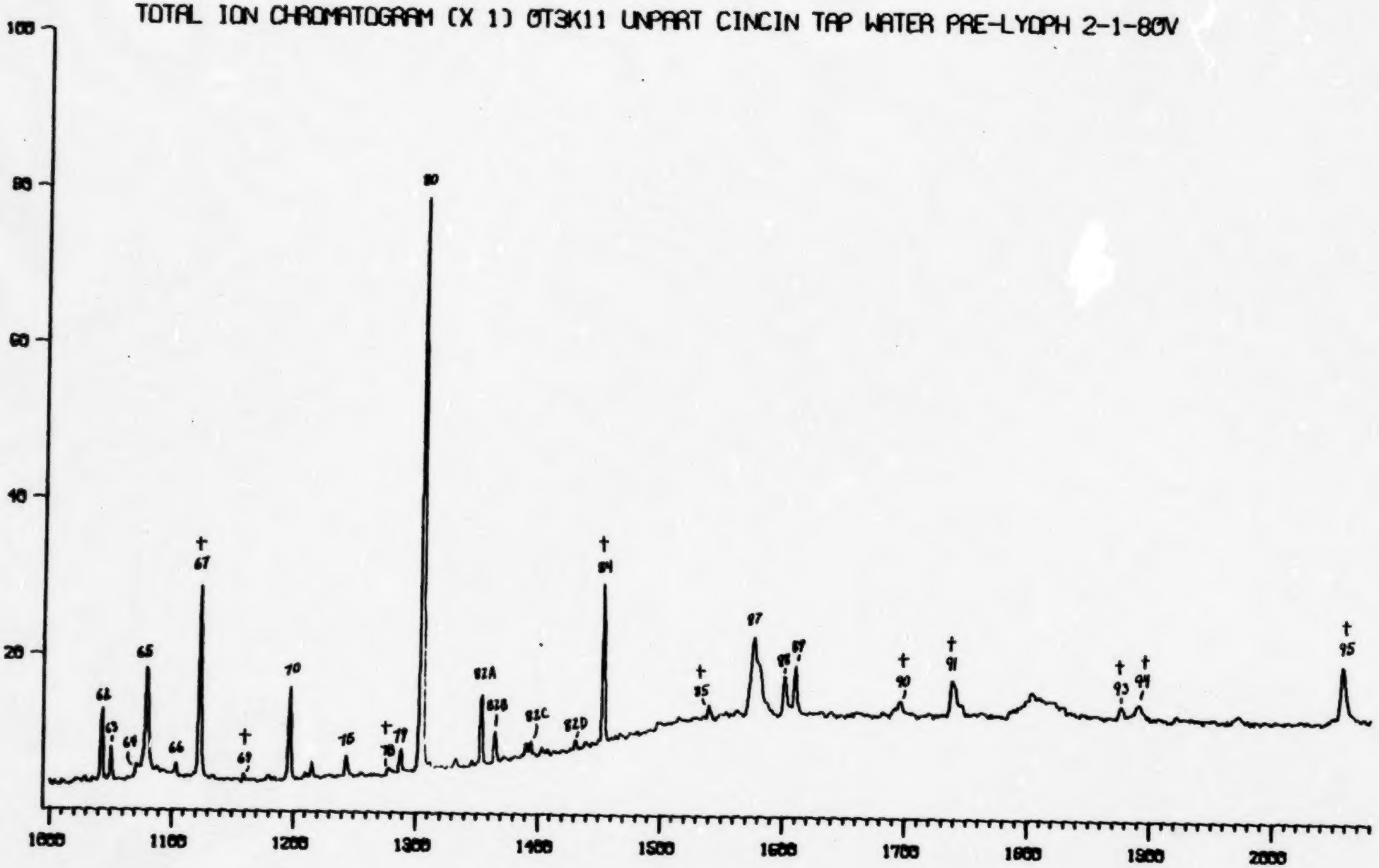

Figure E3. (Continued)

TABLE E3. GC-MS ANALYSIS RESULTS FOR THE UNPARTITIONED ALIQUOT OF THE 10-LITER CINCINNATI TAP WATER SAMPLE, T3K

Sequence[a]	Spectrum Number	RT	RRT	Compound Name[b]	MW	%IS[c]	Relative Retention Times[d] 2T3K1	Relative Retention Times[d] 9T3K12
1	10-8	8.771	0.135	2-methyl propanenitrile	69	125		
2	18-15	9.253	0.142	chloroform	118	660		
4	35-33	10.253	0.158	toluene	92	75		
14	111-108	14.548	0.224	p-xylene plus BP 43; m/e 41, 69, 68	106	95		.162
15	127-123	15.430	0.237	m-xylene	106	40		.176
16	142-139	16.255	0.250	bromodichloromethane	162	825		.185
19	160-158	17.251	0.265	2,6-dimethyl-4-heptanone	142	15		.209
20	171-169	17.853	0.275	5-methyl-2-hexanone	114	50		(.221)
21	174-178	18.016	0.277	o-xylene	106	30		(.221)
22	199-195	19.380	0.298	1,1-dichloro-2-propanone	126	35		
23	209-206	19.923	0.307	1-chloro-2-propanone	92	35		
24	260-259	22.666	0.349	styrene	104	11		.307
25	290-287	24.273	0.373	1,2,4-trimethylbenzene	120	20		.334
26	300-297	24.810	0.382	cyclohexanone	98	35		
27	310-306	25.348	0.390	dibromochloromethane	206	990		.355
30	369-366	28.503	0.439	bromobenzene - D5, IS plus				.407
				a tetrachloro propane(tentative)		90		.409
31	403-399	30.311	0.466	1-(dichloromethyl)naphthalene	210	25		.440
32	411-409	30.736	0.473	BP 74; m/e 84, 82, 76, 47; aberant spectrum?				
33	431-428	31.798	0.489	BP 43; m/e 83, 56, 141				
34	442-439	32.383	0.498	2-butoxy ethanol	118	41		(.477)
35	459-456	33.288	0.512	chloroacetonitrile plus	75	9		
				m-dichlorobenzene	146	3		.489
36	484-481	34.615	0.533	2-cyclohexen-1-one plus MW 98	96	20		.510
37	496-493	35.255	0.542	bromoform	250	115		.523
38	510-508	36.010	0.554	chlorinated				.535
39	527-523	36.910	0.568	2-cyclohexen-1-ol	98	20		
42	553-550	38.290	0.589	2-ethyl-1-hexanol	130	65		
44	573-571	39.353	0.605	2,5-hexanedione	114	10		(.590)
45	596-593	40.575	0.624	benzaldehyde	106	105		.610
49	695-693	45.821	0.705	benzonitrile	103	22		.693
50	733-730	47.835	0.736	BP 69; m/e 41, 42, 54, 68				
51	749-745	48.686	0.749	4-chlorocyclohexanol	134	83		.738
52	760-756	49.273	0.758	triethylphosphate	182	15		

(continued)

TABLE E3. (continued)

Sequence[a]	Spectrum Number	RT	RRT	Compound Name[b]	MW	%IS[c]	Relative Retention Times[d] 2T3K1	9T3K12
55	834-830	53.220	0.819	p-dibromobenzene - D4, IS		75		.807
56	840-837	53.546	0.824	3,4-dimethyl-2,5-furandione (dimethylmaleicanhydride)	126	50	.87(ME)	
57	847-844	53.923	0.830	nitrobenzene - D5, IS + D0; 12:1		240		.820
58	870-868	55.163	0.849	2-phenyl-2-propanol, mixture	136	11		
59	911-907	57.361	0.882	2(2-butoxy ethoxy)ethanol	162	18	(.876)	
60	967-962	60.376	0.929	hexanoic acid	116	20		
62	1043-1039	64.505	1.001	hexaethylbenzene, IS				
63	1050-1048	64.893	1.007	benzylcyanide	117	45		1.006
64	1071-1067	66.040	1.025	2-ethyl hexanoic acid + MW 136	144	(25)	.33(ME)	
65	1080-1074	66.540	1.032	n-eicosane - D42, IS		155		1.030
66	1104-1101	67.866	1.053	N-cyclohexylidene methanamine	111	20		1.050
67	1123-1118	68.913	1.069	phenol; D0 + D5; 20:1	94	260	1.075	
69	1159-1157	70.900	1.099	octanoic acid? (fatty acid)	144	12	.47(ME)	(1.099)
70	1197-1193	73.000	1.132	BP 60; m/e 92, 166, 122		150		
75	1243-1241	75.558	1.171	tributyl phosphate	266	28		
78	1278-1275	77.511	1.201	nonanoic acid	158	11	.58(ME)	
79	1288-1285	78.073	1.210	chloroform-like spectrum; m/e 83, 85, 87				
80	1305-1298	79.031	1.225	trimethylisocyanurate	171	770		
82A	1353-1350	81.743	1.269	dimethyl terephthalate - D4, IS	95			
82B	1364-1361	82.368	1.276	3-ethyl-4-methyl pyrrole-2,5-dione (ethylmethylmaleimide)	139	45		
82C	1394-1392	84.078	1.302	dimethyl phthalate	194	21		
82D	1430-1428	86.140	1.334	5,6,7,7A-tetrahydro-4,4,7A-trimethyl-2-benzofuranone	180	13		
84	1453-1450	87.468	1.354	diethyl phthalate	222	217		
85	1540-1537	92.600	1.433	a lauric acid	200	18		
87	1582-1592	95.100	1.472	4,8,12-trimethyl-3,7,11-tridecatrienenitrile	231	80		
88	1601-1598	96.231	1.489	4-hydroxy-3-methoxy benzaldehyde	152	55		
89	1610-1606	96.768	1.497	1-nitronaphthalene - D7, IS plus N-phenylacetamide	135	71		1.491
90	1696-1702	101.885	1.576	diisooctyl phthalate	390	25		
91	1746-1751	104.873	1.622	myristic acid	228	50	(1.08(ME))	
93	1876-1873	112.741	1.743	pentadecanoic acid	242	20	(1.17(ME))	

(continued)

TABLE E3. (continued)

Sequence[a]	Spectrum Number	RT	RRT	Compound Name[b]	MW	%IS[c]	Relative Retention Times[d] 2T3K1	9T3K12
94	1891-1885	113.640	1.757	dioctyl phthalate	390	22		
95	2057-2050	123.546	1.909	palmitic acid	256	80	(1.25(ME))	

a) The sequence number is used to label the peaks in the GC-MS chromatogram, Figure E3.

b) ME = methyl ester or methyl ether; IS = internal standard; † = a compound attributable to the 10-liter extraction blank.

c) Size (height) of the GC peak in the GC-MS chromatogram (see a, above) expressed as a percentage of the internal standard, hexaethylbenzene.

c) The values shown are the RRT values at which the compound was detected in the acid and neutral fraction, respectively.

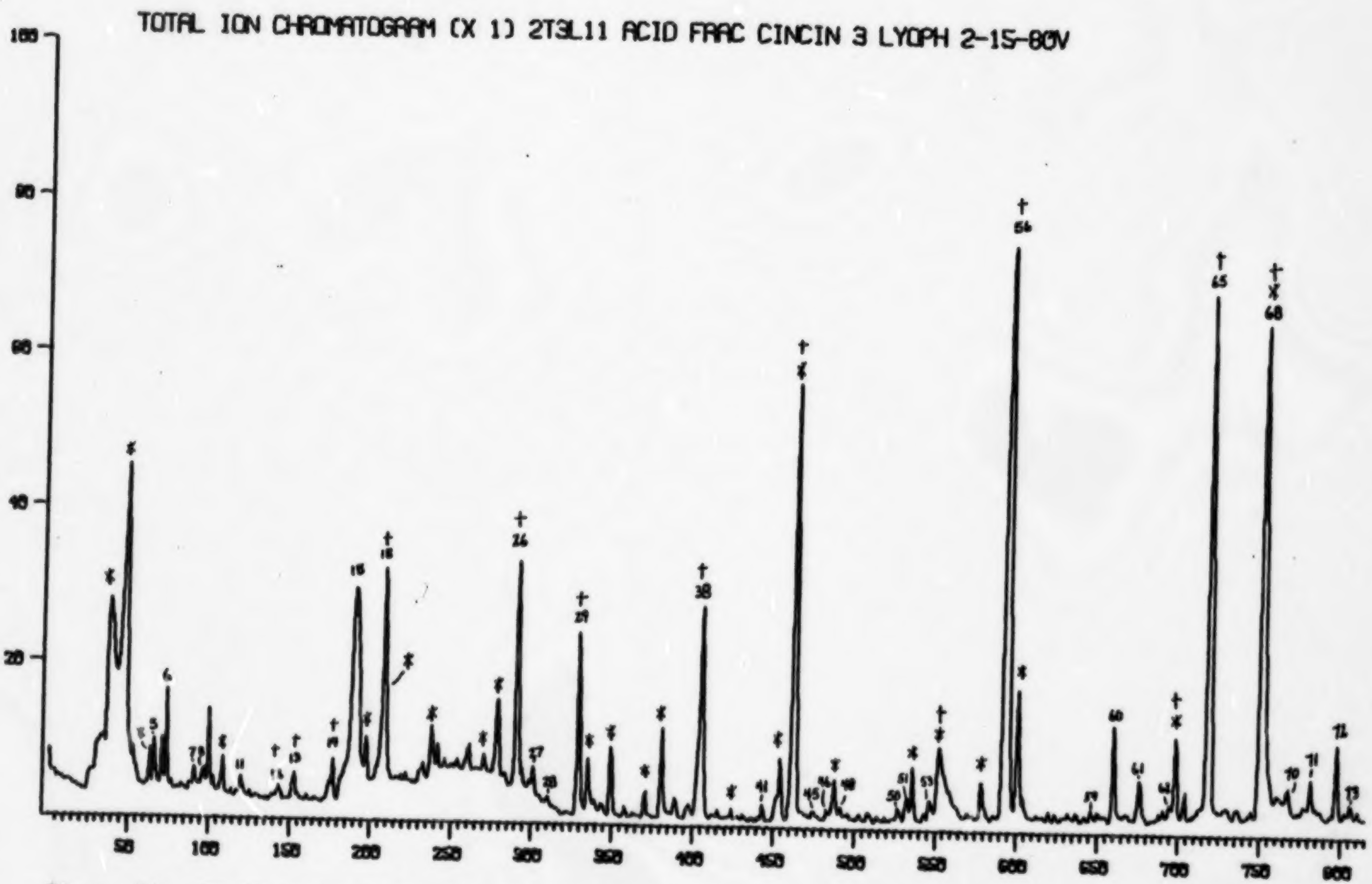

Figure E4. GC-MS analysis results for the acid fraction of the lyophilized 10-liter Cincinnati tap water sample, T3L.

(continued)

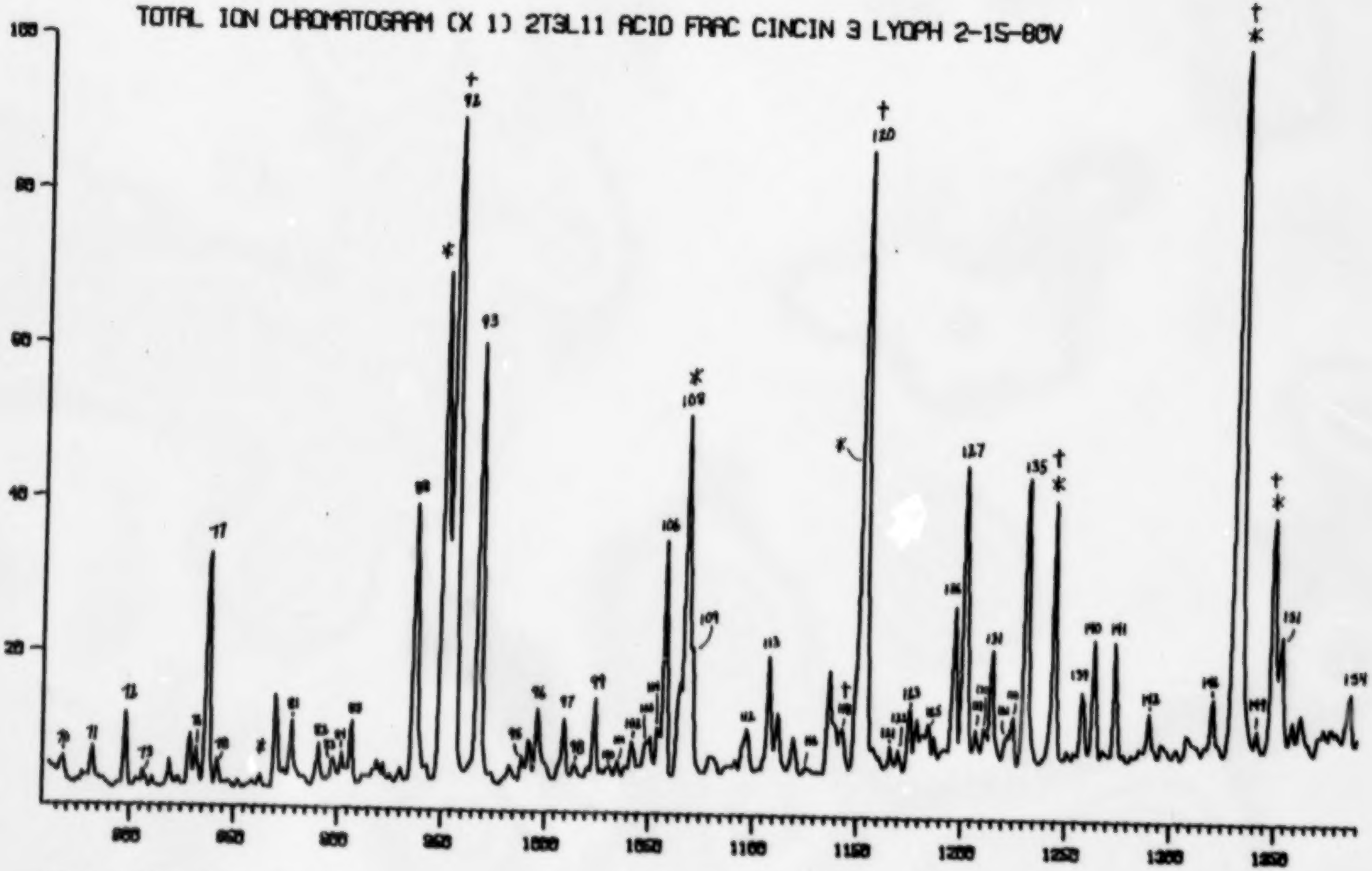

Figure E4. (Continued)

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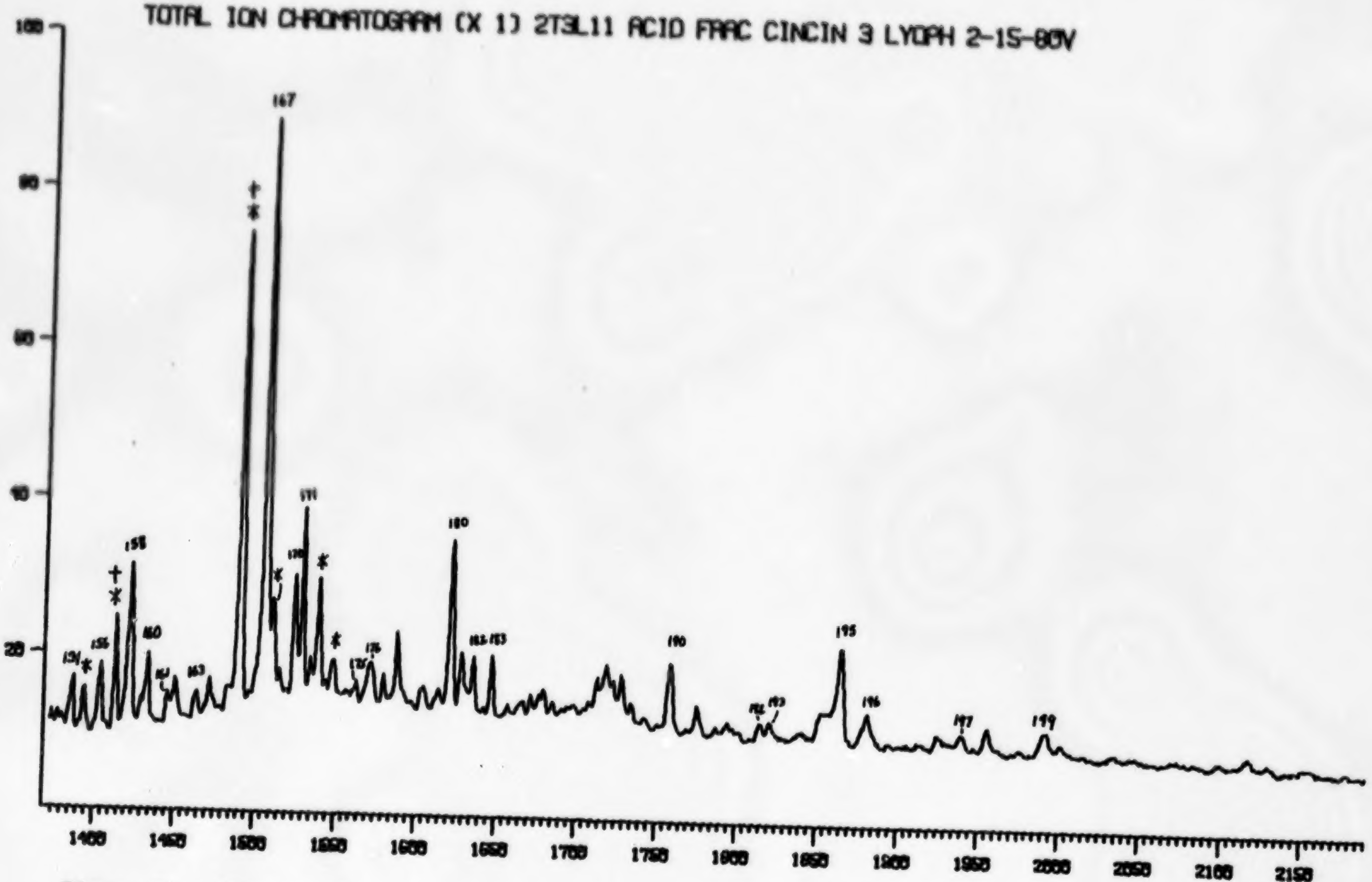

Figure E4. (Continued)

TABLE E4. GC-MS ANALYSIS RESULTS FOR THE ACID FRACTION OF THE LYOPHILIZED 10-LITER CINCINNATI TAP WATER SAMPLE, T3L

Sequence[a]	Spectrum Number	RT	RRT	Compound Name[b]	Molecular Formula	Molecular Weight	GC Peak[c] Size % IS	RS	Match[d]	Proof[e]
5	66-65	10.098	0.155	2,2-dimethyl-1-butanol	C6.H14.O1	102	7	3	812	C
6	74-72	10.540	0.162	similar to #5			25	3		
7	91-87	11.458	0.176	2-ethyl-3-propyl oxirane	C7.H14.O1	114	6	2	923	C
8	97-94	11.781	0.181	3-ethyl-2,2-dimethyl oxirane	C6.H12.O1	100	5	2	832	C
11	120-116	13.035	0.201	4-methyl-2-pentanone	C6.H12O1	100	5	2	955	B
12	143-138	14.321	0.220	†p-xylene + methyl vinyl mercury	C8.H10 C3.H6.HG	106 244	4 4	1 1	man man	B B
13	153-149	14.900	0.229	†m-xylene + 4-heptanone	C8.H10 C7.H14.O1	106 114	8 8	2 2	man 965	B B
14	175-170	16.160	0.249	†1-methoxy-2-propanol	C4.H10.O2	90	12	2	925	B
15	188-182	16.863	0.260	similar to #14			59	4		
18	207-204	17.900	0.275	†hexanoic acid, ME	C6.H12.O2	116	65	4	881	A
26	290-287	22.243	0.342	†2-ethylhexanoic acid, ME	C8.H16.O2	144	62	4	872	A
27	301-296	22.818	0.351	2-t-butyl-3-ethyl oxirane	C8.H16.O	114	8	2	877	B
28	310-307	23.285	0.358	an alkane			3	1		
29	329-325	24.275	0.373	†heptanoic acid, ME	C7.H14.O2	130	49	4	869	B
38	405-400	28.248	0.435	†phenol, ME-D5, IS + DO	C6.H6.O	94	57			A
41	443-438	30.240	0.465	2-methyl-2-propylhexanoic acid, ME	C10.H20.O2	172	4	2	918	C
45	475-472	31.923	0.491	2-acetyl-3-methyl butanoic acid, ME	C7.H12.O3	144	2	1	924	B
46	483-479	32.345	0.498	2-methoxy 10-undecenoic acid, ME	C12.H22.O3	214	3	1	783	D
48	491-493	32.773	0.504	o-cresol, ME m-dichlorobenzene	C7.H8.O1 C6.H4.O2	108 146	3 3	1 1	944 944	B A
50	527-525	34.683	0.534	p-cresol, ME	C7.H8.O1	108	4	2	997	A
51	536-530	35.003	0.539	m-cresol, ME + fatty acid, ME	C7.H8.O1	108	6	2		
53	547-545	35.751	0.550	3,3-dimethyl-2-isopropylbutanoic acid, ME	C9.H18.O2	158	6	2	868	B
56	596-597	38.345	0.590	nonanoic acid, ME	C9.H18.O2	158	156	5	895	A
59	646-644	41.040	0.631	a fatty acid, ME			3	1		
60	660-656	41.796	0.643	isocapric acid, ME	C12.H20.O2	172	11	3	man	C
61	676-672	42.660	0.656	anteisocapric acid, ME	C10.H20.O2	172	11	3	man	C
62	694-692	43.636	0.671	levulinic acid, ME	C5.H8.O3	116	5	2	962	A
65	717-714	44.893	0.691	†capric acid, ME	C10.H20.O2	172	143	5	880	A
68	750-747	46.685	0.718	benzoic acid, ME-D5, IS + DO	C7.H6.O2	122	133			A
70	768-765	47.671	0.733	p-t-butyl phenol, ME	C10.H14.O	150	8	2	957	B
71	782-779	48.443	0.745	iso-undecanoic acid, ME	C11.H22.O2	186	10	3	man	C
72	798-793	49.325	0.759	anteiso-undecanoic acid, ME	C11.H22.O2	186	22	3	man	C

(continued)

TABLE E4. (continued)

Sequence[a]	Spectrum Number	RT	RRT	Compound Name[b]	Molecular Formula	Molecular Weight	GC Peak[c] Size %	IS	RS	Match[d]	Proof[e]
73	806-804	49.766	0.766	p-isopropenylphenol, ME	C9.H10.O1	134		4	2	995	B
76	832-830	51.205	0.788	o-toluic acid, ME	C8.H8.O2	136		11	2	972	A
77	837-835	51.483	0.792	undecanoic acid, ME	C11.H22.O2	186		64	4	808	A
78	842-840	51.758	0.796	similar to #77				7	2		
81	878-875	53.763	0.827	m-toluic acid, ME	C8.H8.O2	136		19	3	937	A
82	891-887	54.491	0.838	p-toluic acid, ME	C8.H8.O2	136		12	3	887	A
83	898-894	54.885	0.844	C12-fatty acid, ME				8	2		
84	902-900	55.110	0.848	C12-fatti acid, ME				8	2		
85	907-904	55.390	0.852	phenyl acetic acid, ME	C8.H8.O2	136		18	2	846	A
88	936-932	57.026	0.877	2,3-dimethyl maleic acid, di-ME	C6.H8.O4	144		76	4	man	A
92	957-959	58.188	0.895	†lauric acid, ME	C12.H24.O2	200		183	5	822	A
93	967-963	58.758	0.904	2-ethyl-3-methyl maleic acid, di-ME	C7.H10.O4	158		120	5	982	B
95	989-986	60.011	0.923	fatty acid, ME				8	2		
96	996-995	60.413	0.929	hydrocinnamic acid, ME	C9.H10.O2	150		20	3	988	A
97	1009-1004	61.161	0.941	isotridecanoic acid, ME	C13.H26.O2	214		18	3	man	B
98	1015-1012	61.506	0.946	o-methyl phenylacetic acid, ME	C9.H10.O2	150		5	2	man	C
99	1024-1020	62.025	0.954	anteisotridecanoic acid, ME	C13.H26.O2	214		22	3	man	B
100	1031-1028	62.428	0.960	p-isopropyl benzoic acid, ME	C10.H12.O2	164		3	1	909	A
101	1035-1033	62.661	0.964	2,4,6-trimethyl benzoic acid, ME	C10.H12.O2	164		5	2	942	A
102	1041-1040	63.011	0.969	an alcohol				10	2		
103	1049-1045	63.476	0.977	a fatty acid, ME				11	2		
104	1054-1053	63.766	0.981	a fatty acid, ME				12	2		
106	1059-1061	64.055	0.985	tridecanoic acid, ME	C13.H26.O2	214		64	4		A
108	1067-1061	64.531	0.993	hexamethylbenzene, IS				100			
109	1071-1074	64.765	1.003	4-oxo-nonanoic acid, ME	C9.H16.O3	172		100	3	986	B
112	1097-1093	66.290	1.026	4-methyl-2-acetobenzoic acid, ME	C10.H10.O3	178		12	3	man	D
113	1108-1104	66.958	1.036	isomyristic acid, ME	C14.H28.O2	228		33	4		A
116	1126-1124	68.073	1.054	2,4,5-trimethylbenzoic acid, ME	C10.H12.O2	164		2	1	946	A
118	1143-1146	69.080	1.069	†phenol essentially no D5	C6.H6.O	94		13	3	996	A
120	1155-1157	69.776	1.080	†myristic acid, ME, partially in the blank	C14.H28.O2	228				954	A
121	1166-1163	70.428	1.090	similar to #109				7	2		
122	1170-1168	70.665	1.093	suberic acid, di-ME	C8.H14.O4	174		6	2	948	A
123	1175-1172	70.960	1.098	an unsaturated fatty acid				17.5	3		

(continued)

TABLE E4. (continued)

Sequence[a]	Spectrum Number	RT	RRT	Compound Name[b]	Molecular Formula	Molecular Weight	GC Peak[c] Size X	IS	RS	Match[d]	Proof[e]
125	1184-1186	71.493	1.106	C15-fatty acid							
126	1197-1192	72.263	1.118	3,4-dichlorobenzoic acid, ME	C7.H4.O2.CL2	190	42		4	843	B
127	1200-1199	72.441	1.121	2,5-dimethylbenzene butyric acid, ME	C12.H16.O2	192	78		4		B
129	1207-1205	72.851	1.127	3-hydroxycapric acid, ME	C10.H20.O3	188	6		2		A
130	1211-1209	73.088	1.131	3,5-dimethyl phenol	C8.H10.O1	122	7		2	815	C
131	1215-1212	73.330	1.134	anteisopentadecanoic acid, ME	C15.H30.O2	242	30		3		A
132	1222-1219	73.755	1.141	2-ethyl-6-hydroxybenzoic acid, ME	C9.H10.O3	166	8		2	982	B
133	1225-1219	73.933	1.144	4-methoxybenzoic acid, ME	C8.H8.O3	152	13		3	964	A
135	1233-1236	74.406	1.151	BP 75, m/e 55, 71, 95, 147							
139	1258-1255	75.911	1.174	clofibric acid, ME	C10.H11.O3.CL	214	19		3	991	A
140	1264-1260	76.273	1.180	azelaic acid, di-ME	C9.H16.O4	188	33		4	983	A
141	1274-1271	76.875	1.189	9-oxyo-capric acid, ME	C10.H18.O3	186	31		4	971	B
142	1290-1286	77.840	1.204	isopalmitic acid, ME	C16.H32.O2	256	13		3		A
146	1321-1318	79.728	1.233	similar to #135			16		3		
149	1342-1340	81.001	1.252	4-chloro-3-methyl phenol	C7.H7.O.CL	142	6		2	820	C
151	1354-1357	81.740	1.264	palmitelaidic acid, ME	C16.H30.O2	254	33		3	man	B
154	1387-1382	83.780	1.295	anteisoheptadecanoic acid, ME	C17.H34.O2	270	14		3		A
156	1404-1398	84.833	1.311	similar to #135			19		3		
158	1421-1416	85.898	1.328	pentachlorophenol, ME	C6.H1.O.CL5	264	44		4	982	A
160	1433-1426	86.661	1.340	undecanedioic acid, di-ME	C11.H18.O4	216	19		3		A
161	1445-1443	87.420	1.351	similar to #160							
163	1463-1459	88.565	1.369	1 chlorine + 1 bromine, aromatic, MW 294					3		
167	1503-1498	91.111	1.408	oleic acid, ME	C18.H34.O2	282	162		5		C
170	1524-1520	92.451	1.429	3,4-dihydroxyacetophenone-DI, ME + BP 151 m/e 194	C8.H8.O3	152	33		4		A
171	1529-1526	92.770	1.434	4(1,5-dimethyl-3-oxohexyl)cyclohexanecarboxylic acid, ME	C15.H26.O3	254	51		4	983	B
175	1563-1565	94.966	1.467	nonadecanoic acid, ME	C19.H38.O2	298	5		2	830	A
176	1572-1577	95.561	1.476	dibromo compound (analogue of #163)			12		3		
180	1621-1617	98.751	1.526	4(1,5-dimethyl-3-oxohexyl)1-cyclohexenecarboxylic acid, ME	C15.H24.O3	252	45		4	834	B
182	1636-1632	99.723	1.541	t-butylphenoxy methanol acetate	C13.H18.O3	222	17		3	879	C
183	1647-1643	100.443	1.552	eicosanoic acid, ME	C20.H40.O2	312	17		3		A
190	1758-1753	107.706	1.663	similar to #180			19		3		
192	1815-1811	111.441	1.721	2,4'-dihydroxydiphenyl methane, di-ME	C13.H12.O2	200	5		2	914	C

(continued)

TABLE E4. (continued)

Sequence[a]	Spectrum Number	RT	RRT	Compound Name[b]	Molecular Formula	Molecular Weight	GC Peak[c] Size % IS	 RS	Match[d]	Proof[e]
193	1821-1818	111.836	1.727	secondary fatty alcohol			6	2		
195	1865-1859	114.730	1.771	BP 205, MW 220, m/e 189, 173, 145						
196	1880-1871	115.716	1.787	a fatty acid, ME			10	2		
197	1940-1935	119.670	1.847	a fatty dicarboxylic acid, di-ME			4	1		
199	1992-1982	123.076	1.900	similar to #192			8	2		

a) The sequence number is used to label the peaks in the GC-MS chromatogram, Figure E4.

b) ME = methyl ester or methyl ether; IS = internal standard; † = a compound attributable to the 10-liter extraction blank.

c) Size (height) of the GC peak in the GC-MS chromatogram (see a, above) expressed as: %HEB, a percentage of the internal standard, hexaethylbenzene; RS, the relative size parameter explained in Section 5.

d) The quality index of the computer mass spectral library match (Finnigan INCOS software) where the value 1000 reflects a perfect fit of the data mass spectrum with the library mass spectrum.

e) Proof reflects the confidence level of the analyst: A, confirmed identification by comparison to data from a standard; B, highest confidence level for non-confirmable compounds; C, less than 80% confidence level; D, less than 50% confidence level.

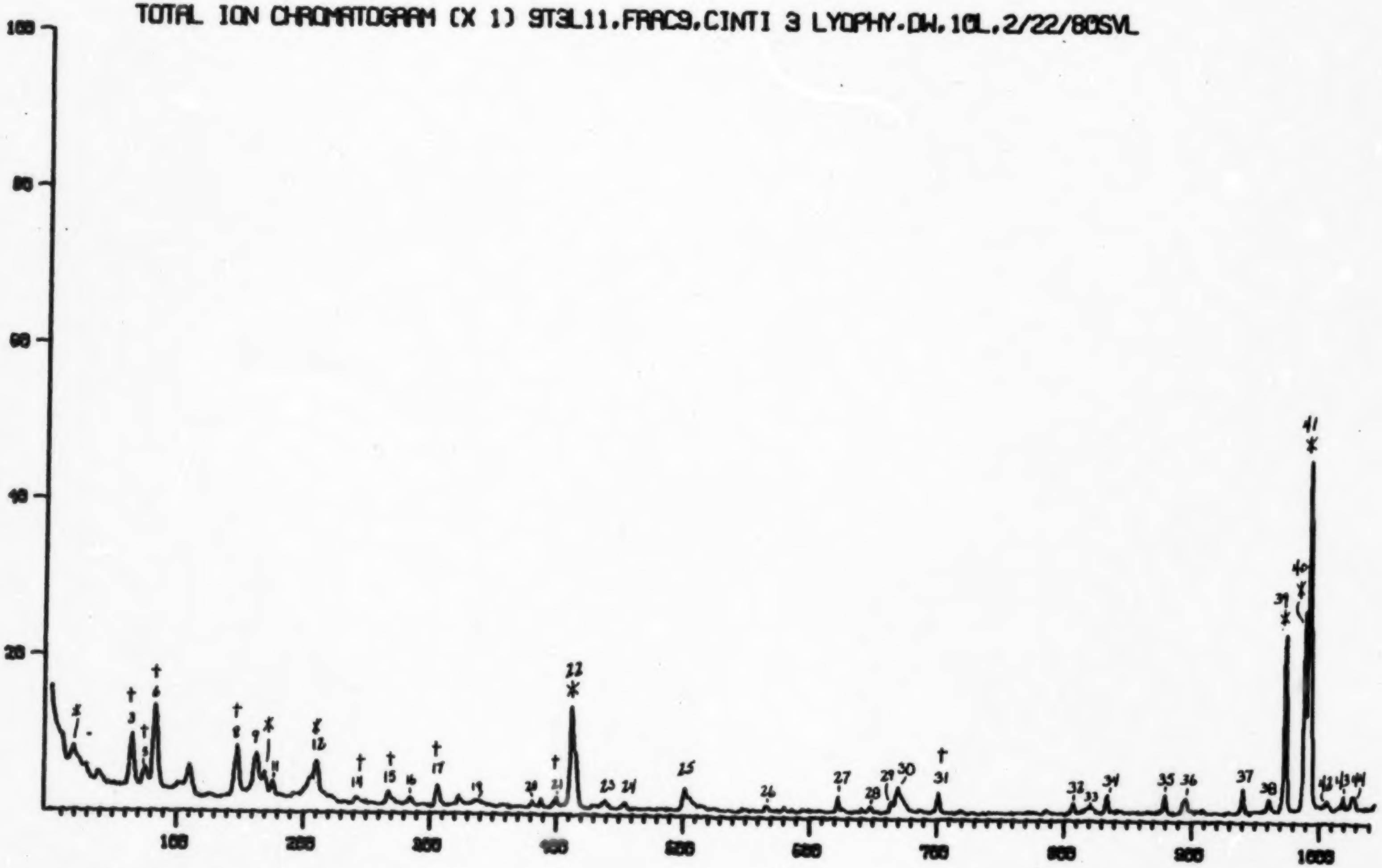

Figure E5. GC-MS analysis results for the aromatic/medium polarity fraction of the lyophilized 10-liter Cincinnati tap water sample, T3L.

(continued)

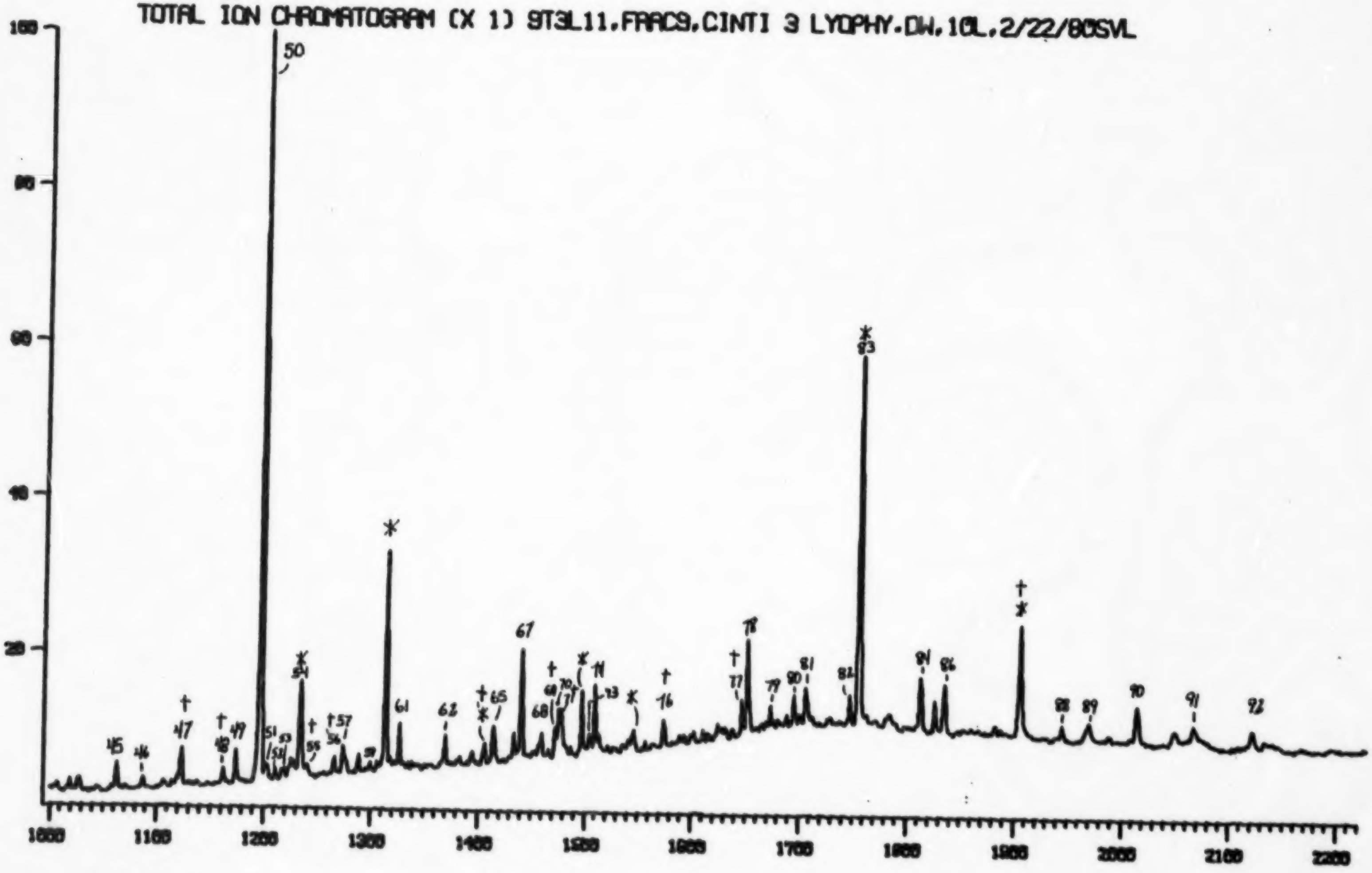

Figure E5. (Continued)

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TABLE E5. GC-MS ANALYSIS RESULTS FOR THE AROMATIC/MEDIUM POLARITY FRACTION OF THE LYOPHILIZED 10-LITER CINCINNATI TAP WATER SAMPLE, T3L

Sequence[a]	Spectrum Number	RT	RRT	Compound Name[b]	Molecular Formula	Molecular Weight	GC Peak[c] Size %	IS	RS	Match[d]	Proof[e]
3	64-59	9.301	0.143	†ethylbenzene	C8.H10	106		7	2	997	A
5	75-70	9.855	0.152	†p-dimethylbenzene	C8.H10	106		3	1	985	A
6	83-79	10.258	0.158	†m-dimethylbenzene	C8.H10	106		11	3	978	A
8	148-141	13.475	0.207	†o-dimethylbenzene	C8.H10	106		7	2	987	A
9	163-155	14.223	0.219	1-methyl-4-isopropenyl cyclohexene	C10.H16	136		5	2	986	C
11	176-173	14.868	0.229	4-methylene-1-(1-methylethyl)cyclohexene	C10.H16	136		2	1	963	C
12	205-196	16.291	0.251	mixture 4-methyl-2-pentanol + p-ethyltoluene	C6.H14.O C9.H12	102 120		4.5 4.5	2 2	932 man	A A
14	243-237	18.138	0.279	†1,3,5-trimethylbenzene	C9.H12	120		1	1	981	A
15	268-263	19.351	0.298	†styrene	C8.H8	104		2	1	978	B
16	285-280	20.181	0.310	p-cymene	C10.H14	134		1	0	991	A
17	306-301	21.193	0.326	†1,2,4-trimethylbenzene	C9.H12	120		3	1	990	A
19	338-327	22.745	0.350	dibromochloromethane	C .H1.CL1.BR2	206		1	0	man	A
20	381-376	24.810	0.328	5-ethyl-1,3-dimethylbenzene	C10.H14	134		1	0	986	A
21	400-395	25.726	0.396	†1,2,3-trimethylbenzene	C9.H12	120		1.5	1	985	A
22	412-407	26.313	0.405	bromobenzene-D5, IS							
23	440-447	27.673	0.426	4-ethyl-1,3-dimethylbenzene	C10.H14	134		1	0	802	A
24	454-450	28.346	0.436	4-ethyl-1,2-dimethylbenzene	C10.H14	134		1	0	851	A
25	501-496	30.576	0.470	silicone				3	1		
26	566-560	33.688	0.518	1,2,3,5-tetramethylbenzene	C10.H14	134		1	0	976	A
27	622-616	36.368	0.560	siloxane			2	1			
28	647-643	37.563	0.578	1,2,3,4-tetramethylbenzene	C10.H14	134	1	0		931	A
29	664-660	38.381	0.590	a C2 styrene + an alkane			1.5	1			
30	669-658	38.628	0.594	2-decen-1-ol	C10.H20.O	156	3.5	1		948	D
31	701-695	40.181	0.618	†benzaldehyde	C7.H6.O	106	3	1		970	A
32	807-801	45.246	0.696	alkane			2	1			
33	821-826	45.928	0.707	a fatty aldehyde			1	1			
34	834-830	46.561	0.716	siloxane			2.5	1			
35	880-874	48.791	0.751	acetophenone	C8.H8.O	120	2.5	1		957	A
36	895-898	49.520	0.762	alkane			2	1			
37	941-933	51.773	0.797	alkane			3	1			
38	961-956	52.763	0.812	a fatty aldehyde			2	1			
39	974-967	53.415	0.822	dibromobenzene-D4, IS			23				
40	989-984	54.175	0.833	nitrobenzene-D5, IS							

(continued)

TABLE E5. (continued)

Sequence[a]	Spectrum Number	RT	RRT	Compound Name[b]	Molecular Formula	Molecular Weight	GC Peak[c] Size % IS	GC Peak[c] Size RS	Match[d]	Proof[e]
41	993-990	54.385	0.837	naphthalene-D8, IS						
42	1006-1012	55.051	0.847	alkane			1.5	0		
43	1019-1014	55.715	0.857	siloxane			2	1		
44	1028-1022	56.173	0.864	alkane			2	1		
45	1062-1060	57.900	0.891	alkane			4	2		
46	1088-1081	59.238	0.911	mixture a fatty aldehyde m/e 203, 218			2	1		
47	1123-1114	61.061	0.939	†2-methylnaphthalene	C11.H10	142	4	2	994	A
48	1162-1158	63.118	0.971	†1-methylnaphthalene	C11.H10	142	2	1	969	A
49	1174-1169	63.756	0.981	alkane			5	1		
50	1197-1189	65.015	1.000	hexaethylbenzene, IS			100			
51	1202-1207	65.296	1.004	a fatty aldehyde			2	1		
52	1211-1207	65.788	1.012	(1-pentylheptyl)benzene	C18.H30	246	2	1	933	C
53	1218-1213	66.173	1.018	2-chloroaniline	C6.H6.N.CL	127	1.5	1	915	C
54	1234-1230	67.051	1.031	n-eicosane-D42, IS						
55	1241-1247	67.441	1.037	†2,6-dimethylnaphthalene + dichloroaniline	C12.H12 C6.H5.N.CL2	156 161	2 2	0 0	948 man	A C
56	1266-1263	68.818	1.509	†biphenyl	C12.H10	154	2	1	992	A
57	1274-1270	69.261	1.065	alkane			4	1		
59	1300-1296	70.708	1.088	alkane			1.5	1		
61	1327-1324	72.233	1.111	possibly C5.H6.CL6 MW 276 hexachloropentane			5.5	2		
62	1370-1365	74.656	1.148	alkane			4.5	2		
65	1415-1411	77.215	1.188	4-hydroxy-3,3,5,5-tetramethylcyclohexanone	C10.H18.O2	170	5	2	853	D
67	1441-1437	78.708	1.211	pentylbenzoate	C12.H16.O2	192	13	3	975	C
68	1459-1455	79.755	1.227	alkane			3	1		
69	1472-1469	80.510	1.238	†2,3-dihydro-1,1,3-trimethyl-3-phenyl-(1H)-indene	C18.H20	236	4	1	989	C
70	1476-1469	80.745	1.242	MW 182 + MW 196 alkylated aromatic			2	1		
71	1478-1482	80.863	1.244	†methylpalmitate	C17.H34.O2	270	1	2	966	A
73	1504-1502	82.390	1.267	mixture chlorinated MW 282 + 1,2-dimethyl-4-(phenylmethyl)benzene	C15.H16	196	2	1	942	B
74	1509-1507	82.686	1.272	ethyl palmitate	C18.H36.O2	284	8.5	2	888	A
76	1574-1571	86.513	1.331	†fluorene	C13.H10	166	4	1	981	A
77	1646-1643	90.791	1.397	†methyl stearate	C19.H38.O2	298	5	2	man	A
78	1651-1649	91.090	1.401	4-phenyl-bis-cyclohexane	C18.H26	242	13	3	967	B

(continued)

TABLE E5. (continued)

Sequence[a]	Spectrum Number	RT	RRT	Compound Name[b]	Molecular Formula	Molecular Weight	GC Peak[c] Size % IS	GC Peak[c] Size RS	Match[d]	Proof[e]
79	1673-1671	92.406	1.421	ethyl stearate	C20.H40.02	312	2	1	man	A
80	1695-1691	93.721	1.442	similar to #78			4	2		
81	1706-1704	94.376	1.452	similar to #78			5	2		
82	1747-1742	96.820	1.489	similar to #78			4	2		
83	1755-1751	97.298	1.497	1-nitronaphthalene-D7, IS						
84	1813-2395	100.743	1.550	2-phenylpropanone	C9.H100	134	7.5	2	907	C
86	1836-1831	102.113	1.571	o-terphenyl	C13.H14	230	6	2	man	A
88	1945-1942	108.526	1.669	mixture? tetrachlorobiphenyl	C12.H6.CL4	290	2	1	859	B
89	1970-1962	109.983	1.692	alkylated aromatic			3	1		
90	2015-2009	112.601	1.732	similar to #92			5	2		
91	2067-2063	115.613	1.778	9-methyl anthracene	C16.H12	192	2.5	1	971	A
92	2122-2113	118.775	1.827	diphenylcyclohexane (tentative)	C18.H20	236	3	1	896	C

a) The sequence number is used to label the peaks in the GC-MS chromatogram, Figure E5.

b) ME = methyl ester or methyl ether; IS = internal standard; † = a compound attributable to the 10-liter extraction blank.

c) Size (height) of the GC peak in the GC-MS chromatogram (see a, above) expressed as: %HEB, a percentage of the internal standard, hexaethyl benzene; RS, the relative size parameter explained in Section 5.

d) The quality index of the computer mass spectral library match (Finnigan INCOS software) where the value 1000 reflects a perfect fit of the data mass spectrum with the library mass spectrum.

e) Proof reflects the confidence level of the analyst: A, confirmed identification by comparison to data from a standard; B, highest confidence level for non-confirmable compounds; C, less than 80% confidence level; D, less than 50% confidence level.

APPENDIX F

CONTENTS AND LISTS OF TABLES FOR VOLUMES 1 AND 2

The contents and lists of tables for the other volumes of this report are presented here to aid the reader's grasp of the scope of this report in the absense of these other two volumes.

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